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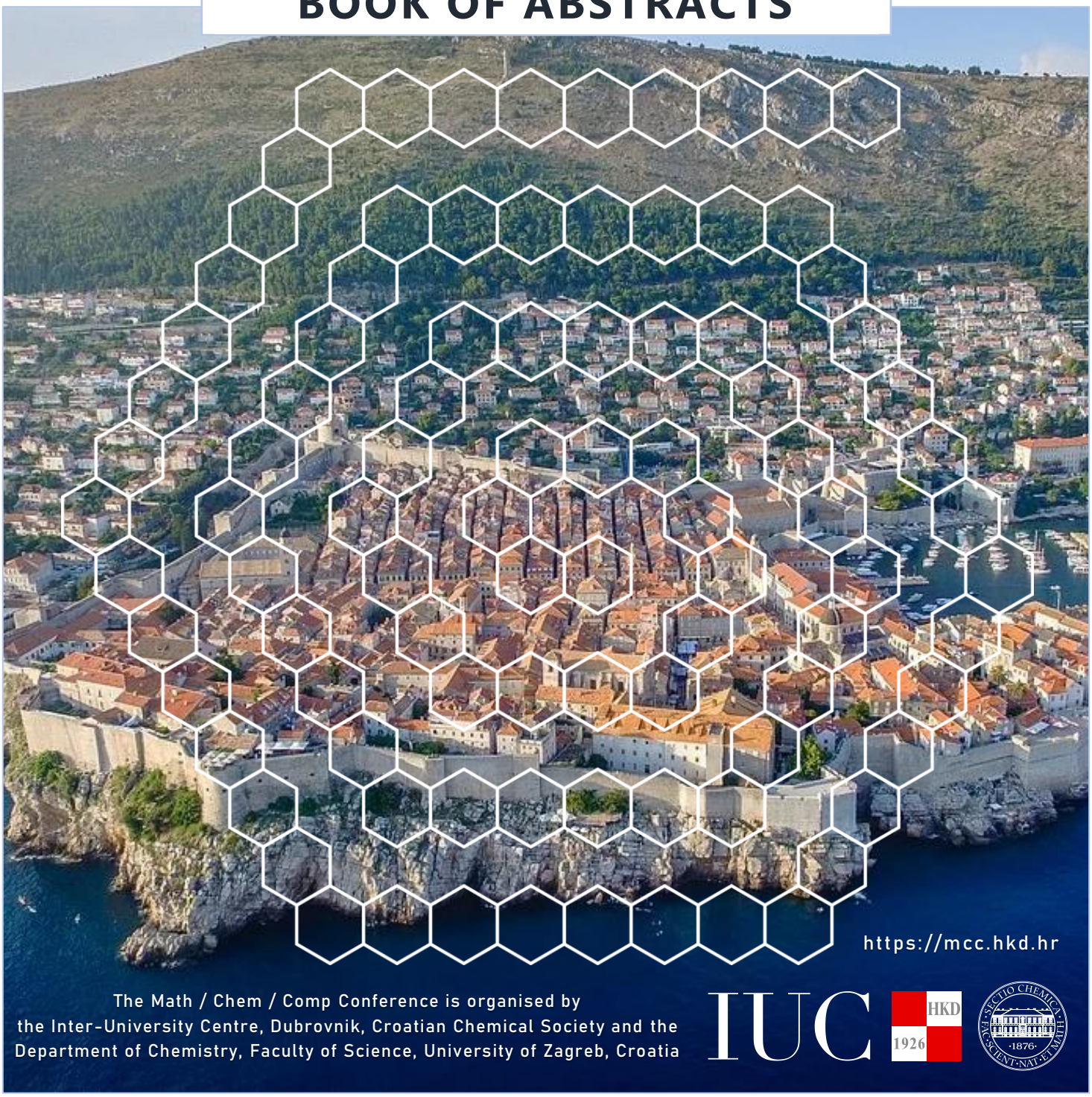
Math/Chem/Comp 2021 – 32nd MC² Conference

Inter University Centre Dubrovnik, 7 – 11 June 2021

BOOK OF ABSTRACTS



The Math / Chem / Comp Conference is organised by
the Inter-University Centre, Dubrovnik, Croatian Chemical Society and the
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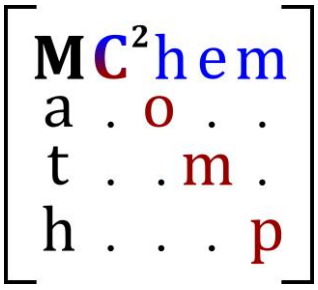

Math/Chem/Comp 2021 – 32nd MC² Conference

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IMPRESSUM

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Zagreb, 2021

The 32nd International Course and Conference on the Interfaces among Mathematics, Chemistry and Computer Sciences: Mathematics, Chemistry, Computing (Math/Chem/Comp, MC^2-32)

Since 1986, the Math/Chem/Comp meetings have been bringing together researchers working on diverse subjects spanning mathematics, computer science, and chemistry. In continuation of this tradition, presentations concerning all aspects of current research on computer modelling, combinatorics, graph theory, and topology applied to any area of chemistry, physics, material and life sciences will be welcomed. The conference program will include invited plenary and special lectures workshops and posters. In particular, the MC^2-32 meeting will revolve around the following topics:

1. Mathematical methods and computational algorithms in modelling of atoms, molecules, and chemical processes;
2. Mathematical chemistry and chemical graph theory;
3. Molecular modelling in practice (including molecular dynamics and aggregation).

In addition, the meeting will involve three special events:

Special session in honour to 90th Birthday of Prof. Milan Randić

Special session in memory of Dr. Mircea Diudea

Workshop in computational chemistry: *Modelling Reactions at Metal-organic Interfaces*
Igor Rončević (Institute of Organic Chemistry and Biochemistry, CAS, Prague, Czech Republic)

This year new modes of presentation have been introduced: apart from *live oral or poster presentation at the conference venue*, it is possible to participate with *live oral presentation via remote connection* (using the Zoom software); *prerecorded oral presentation* (via uploading of a video file) or *silent presentation* (via uploading of the presentation slides or poster in pdf format).

Hrvoj Vančik and Jerzy Cioslowski

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Math/Chem/Comp 2021 – 32nd MC² Conference

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12:00 – 12:15	**COFFEE BREAK**
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LECTURES

REVERSE ENGINEERING IN QUANTUM CHEMISTRY: HOW TO REVEAL THE FIFTH-ORDER OFF-DIAGONAL CUSP IN THE ONE-ELECTRON REDUCED DENSITY MATRIX WITHOUT ACTUALLY CALCULATING IT

Jerzy Cioslowski

Institute of Physics, University of Szczecin, Wielkopolska 15, 70-451 Szczecin, Poland

Three approaches to revealing the presence of the fifth-order off-diagonal cusp in the one-electron reduced density matrix (the 1-matrix) are discussed. The simplest of them is based upon reverse engineering of the previously known properties of natural orbitals and their occupancies. The most straightforward approach that involves explicit evaluation of the 1-matrix is shown to lead to almost intractable algebra. A closed-form expression for the spherical average of $|\mathbf{r}_1-\mathbf{r}|\,|\mathbf{r}_2-\mathbf{r}|$ with respect to the orientation of $\mathbf{r}$ is obtained as a by-product of this investigation.

UNIFORM DESCRIPTION OF THE HELIUM ISOELECTRONIC SERIES DOWN TO THE CRITICAL NUCLEAR CHARGE

Filip Prątnicki

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An efficient computational scheme for calculation of highly accurate ground-state electronic properties of the helium isoelectronic series, permitting uniform description of its members down to the critical nuclear charge Z_c, will be described.[1] It is based upon explicitly correlated basis functions derived from the regularized Krylov sequences (which constitute the core of the free ICI/FC method of Nakatsuji) involving a term that introduces split length scales. For the nuclear charge Z approaching Z_c, the inclusion of this term greatly reduces the error in the variational estimate for the ground-state energy, restores the correct large-r asymptotics of the one-electron density $\rho(Z;r)$, and dramatically alters the manifold of the pertinent natural amplitudes and natural orbitals. The advantages of this scheme will be illustrated with calculations for $Z = 1$ and $Z = Z_c$ carried out with a moderate-size 12th-generation basis set of 2354 functions. For $Z = Z_c$, the augmentation is found to produce a *ca*. 5000-fold improvement in the accuracy of the approximate ground-state energy, yielding values of various electronic properties with between seven and eleven significant digits. Some of these values, such as those of the norms of the partial-wave contributions to the wavefunction and the Hill constant, have not been reported in the literature thus far. The same is true for the natural amplitudes at $Z = Z_c$, whereas the published data for those at $Z = 1$ are revealed by the present calculations to be grossly inaccurate. Approximants that yield correctly normalized $\rho(1;r)$ and $\rho(Z_c;r)$ conforming to their asymptotics at both $r\to 0$ and $r\to\infty$ will be presented.

REFERENCES

[1] J. Cioslowski and F. Prątnicki, *J. Chem. Phys.* 153 (2020) 224106 and the references cited therein.

LINKING ATOMISTIC MODELLING WITH EXPERIMENTAL DATA: GENERAL JAHN-TELLER MODELS FOR DEFECTS IN SEMICONDUCTORS

Gabriela Herrero-Saboya,[a] Layla Martin-Samos,[a] Anne Hemeryck,[b] and Nicolas Richard[c]

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Tuning the electronic properties of semiconductors through point-like defects remains one of the main challenges of modern technology. Beyond controlling the concentration of free carriers across the band gap, the intentional generation of defects in the crystalline structure has proved to present infinite industrial applications (*e.g*. enhancing photon-absorption in silicon-based solar cells [1][2]). Within such technologicallydriven context, a theoretical understanding of the defect properties is ideally required.

When modelling defects in semiconductors one commonly encounters the instability of the degenerate defect electronic states, resulting in a symmetry-breaking which dictates the shape of the Adiabatic Potential Energy Surfaces (APES): the Jahn-Teller effect. *Ab initio* calculations based on the density-functional theory do however often overlook fundamental symmetry considerations, *blindly* targeting the ground state geometries of individual centres for a given set of convergence parameters and functional flavour. In this work, we deepen the understanding of selected defects in silicon (see for example [3]), providing full theoretical pictures based on general frameworks such as Group theory. By explicitly guiding our *ab initio* calculations by such symmetry arguments, we ground the validity of our numerical values and their comparison with experimental data (EPR spectroscopy, Optical Absorption, etc.). More specifically, we target the Minimum Energy Paths between Jahn-Teller distortions, coherently sampling the APES.

REFERENCES

[1] J. Olea, M. Toledano-Luque, D. Pastor, G. González-Díaz, and I. Martín, Journal of Applied Physics, 104, 016105 (2008)
[2] Antonio Luque, Antonio Martín, and Colin Stanley, Nature Photonics 6, 146–152 (2012)
[3] G. Herrero-Saboya, L. Martin-Samos, A. Jay, A. Hemeryck, and N. Richard, Journal of Applied Physics 127, 085703 (2020).

FEW ELECTRON SYSTEMS CONFINED IN GAUSSIAN POTENTIAL WELLS: CONNECTION TO HOOKE ATOMS AND INTRODUCTION TO GAUSSIAN MOLECULAR STRUCTURE

Xabier Telleria-Allika,[a] Jose M. Mercero,[a] Jon M. Matxain,[a,b]
Xabier Lopez,[a,b] and Jesus M. Ugalde[a,b]

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In this work, we have computed and implemented one-body integrals concerning gaussian confinement potentials over gaussian basis functions. Then, we have set an equivalence between gaussian and Hook atoms and we have observed that, according to singlet and triplet state energies, both systems are equivalent for large confinement depth for a series of even number of electrons n = 2,4,6,8 and 10. Unlike with harmonic potentials, gaussian confinement potentials centered a several points give rise to molecular structures which allows us have a much richer versatility when tuning magnetic properties of these quantum systems. In a first approach concerning molecular systems, we have studied homonuclear diatomic gaussian systems by exploring how the ground state epin multiplicity switches from singlet to triple depending on the potential whell depth V_0 and the interatomic distance R keeping the one-centre potential curvature fixed to a given value $0.5\omega^2$.

REFERENCES

[1] Ugalde, J.; Sarasola, C. Evaluation of Screened Nuclear Attraction and Electron Repul-sion Molecular Integrals over Gaussian Basis Functions.International Journal of Quan-tum Chemistry1997,62, 273–278.
[2] Taut, M.Phys. Rev. A1993,48, 3561.
[3] Cioslowski, J.; Strasburger, K.; Matito, E. Benchmark calculations on the lowest-energysinglet, triplet, and quintet states of the four-electron harmonium atom.2014,141,044128.
[4] S. Albeverio, M. G.-L. N., S. Fassari; Rinaldi, F. The Birman-Schwinger Operator for aParabolic Quantum Well in a Zero-Thickness Layer in the Presence of a Two-DimensionalAttractive Gaussian Impurity.Frontiers in Physics2019,7.
[5] J. D. Castańo-Yepes, C. R.-G., D.A. Amor-Quiroz; Gómez, E. Impact of a topological de-fect and Rashba spin-orbit interaction on the thermo-magnetic and optical properties of a2D semiconductor quantum dot with Gaussian confinement.Physica E: Low-dimensionalSystems and Nanostructures2019,109, 59–66

BIG DATA ANALYSIS AND QSAR
FINDING NEEDLES IN A HAYSTACK: DETERMINING KEY MOLECULAR DESCRIPTORS ASSOCIATED WITH THE BLOOD-BRAIN BARRIER ENTRY OF CHEMICAL COMPOUNDS USING MACHINE LEARNING

Claudiu N. Lungu,[1] Subhabrata Majumdar,[2] Subhash C. Basak,[3]
Diudea V. Mircea,[1] and Gregory D. Grunwald[4]

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Big data is a field that establishes ways to analyze, systematically extract information from data sets that are too large or complex to be dealt with by traditional data processing application software. Big data challenges include capturing data, data storage, data analysis, search, sharing, transfer, visualization, querying, updating, information privacy and data source. Big data was originally associated with three key concepts: volume, variety, and velocity. We used two sets of calculated molecular descriptors to predict blood-brain barrier (BBB) entry of a collection of 415 chemicals. The set of 579 descriptors were calculated by Schrodinger and TopoCluj software. Polly and Triplet software were used to calculate the second set of 198 descriptors. Following this, modelling and a two-deep, repeated external validation method was used for QSAR formulation. Results show that both sets of descriptors individually and their combination give models of reasonable prediction accuracy. We also uncovered the effectiveness of a variable selection approach, by showing that for one of our descriptor sets, the top 5 % predictors in terms of random forest variable importance are able to provide a better performing model than the model with all predictors. The top influential descriptors indicate important aspects of molecular structural features that govern BBB entry of chemicals.

QSPR METHOD FOR PREDICTION OF SORPTION PARAMETERS OF LIGHT GASES IN GLASSY POLYMERS

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Problems of predicting physical and chemical properties of substances are an inseparable part of the general problem of the design of materials with desired properties. This report proposes a technical information about a method which was developed for predicting the sorption parameters of most light gases in glassy polymers. Similar problems were investigated in [1-4]. The proposed method consists of several steps. First, realistic conformations of polymer macromolecules (up to 600 atoms) are constructed using the Python RDKit package [5]. For each of obtained conformations a curve is built that relates the "accessible surface area" (*ASA* calculated via the Lee-Richards algorithm) to the radius of this probe, and also seven similar curves, which relate the polarized (neutral, positively or negatively charged, etc.) *ASA* to the radius of the spherical probe that represents the variety of penetrant gases. The linear approximation coefficients of these dependences, averaged between ten conformations for robustness, are used as explanatory variables in a multiple linear regression (adjusted with 5-fold cross-validation procedure). Significant variables and their weights in regression are determined on the basis of experimental measurements (~1800 data points) from the Database [6]. The average relative error is 104% for universal 6-variables regression, and from 56% to 101% for partial regressions built for each specific gas, which is a good result considering large (up to the decimal order) errors of experimental measurements. In comparison with previous versions of this method [7, 8] we considerably fostered the algorithms and the generalization capability of the regression.

REFERENCES

[1] J. W. Barnett, C. R. Bilchak, Y. Wang, B. C. Benicewicz, L. A. Murdock, T. Bereau, S. K. Kumar, *Sci. Adv*. 6 (20) (2020) eaaz4301.
[2] Chen, L.; Pilania, G.; Batra, R.; Huan, T. D.; Kim, C.; Kuenneth, C.; Ramprasad, R. *Materials Science and Engineering R: Reports* 2021, 144, 100595
[3] Yu.Yampolskii, S.Shishatskii, A.Alentiev, K.Loza, *J.Membr.Sci*. 149 (1998) 203–220
[4] V. Ryzhikh, D.Tsarev, A.Alentiev, Yu.Yampolskii, *Journal of Membrane Science* 487 (2015) 189–198
[5] RDKit: Open-source cheminformatics; http://www.rdkit.org
[6] A. Alentiev, Yu. Yampolskii, V. Ryzhikh, and D. Tsarev, *Pet. Chem*. 53, 554 (2013).
[7] Goubko M., Miloserdov O., Yampolskii Yu., Ryzhikh V., *Polymer Science*. 2019. V. 61, Issue 5. 718–732.
[8] Miloserdov, O., *Adv Syst Sci Appl*, 20(3) (2020) 91-104.

A SHAPE MATCHING ALGORITHM FOR OFF-LATTICE ATOM RESOLVED KINETIC MONTE CARLO

Miha Gunde,[a] Nicolas Salles,[b] Anne Hemeryck,[c] and Layla Martin-Samos[d]

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Kinetic Monte Carlo (kMC) is a multi-scale computational approach which simulates evolution of a system by propagating a set of small-scale events, given by their initial and final configurations, and a probability of event occurrence. A basic process of kMC is to parse the system of simulation and associate possible events from a catalogue of events to system sites. The task is to compare the local environment around a system site to initial configuration of an event. An event is associated to a site if the local environment around it is similar to the initial configuration of an event. Once all system sites are parsed, the kMC algorithm chooses a site to execute the given associated event. At this stage, the task is to find the exact rigid transformation of the event configuration such that it matches to the local environment at the chosen system site. Such rigid transformations are translation, rotation, reflection, and atom index permutation. Once the correct rigid transformation is found, the event is executed by applying event final configuration to the local environment around chosen system site.

In this work, we propose a shape-matching algorithm specific to the described situation in kMC. At the stage of event-site identification it is aided by simple graph isomorphism, while at the stage of finding rigid transformations it assumes no prior knowledge of atomic assignments, and is able to find the proper rigid transformations. The algorithm outline will be presented and some specific examples of kMC simulations shown.

ARTN AS A PLUGIN FOR ELECTRONIC STRUCTURE CALCULATION AND MOLECULAR DYNAMICS CODES

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One of the main drawbacks of present saddle point and minimum energy pathway (MEP) semi-automatic finders is the need to identify an initial and a final configuration. In complex cases, as for instance in the oxidation of silicon, the human workload to guess final configurations becomes so demanding that it often precludes the identification of new and meaningful mechanisms. The Activation Relaxation Technique nouevau (ARTn), developed some years ago by N. Mousseau [1], provides a means of circumventing this issue. However, its current implementation [2], requires considerable modifications to the software to be used with different force and energy engines, which has precluded its massive adoption. We present a redesign of the workflow of ARTn so that it functions as a plugin to energy and force engines instead of as a standalone code; the main idea being that it is the engine that calls ARTn and not ARTn that calls a specific engine. Ideally this should allow easier integration of the algorithm in classical molecular dynamics codes and electronic structure calculation packages. The essence of the revised algorithm workflow as implemented in the Quantum ESPRESSO suite for electronic structure calculations [3] will be summarized and for a few selected simple examples its usage and efficiency with respect to currently implemented MEP semi-automatic finders, such as the nudged elastic band (NEB) method, will also be addressed.

REFERENCES

[1] G. T. Barkema and N. Mousseau, *Phys. Rev. Lett.* 77, (1996) 4358.
[2] A. Jay *et al.*, *J. Chem. Theory Comput.* 16, (2020), 6726.
[3] P. Gianozzi *et al.*, *J. Phys.: Condens. Matter* 29, (2017), 465901.

MACHINE LEARNING MULTIVARIATE LINEAR REGRESSION: EVALUATING ALL POSSIBLE REGRESSION MODELS

Tomica Hrenar

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Extensive parallelized machine learning procedure was implemented [1] and applied for the generation of all possible multivariate linear regression (MLR) models for any type of real data. MLR models were constructed from the linear combination of original variables as well as their higher-order terms (including couplings) up to the arbitrary polynomial degree *i*. MLR was performed using the following expression for matrices of coefficients ***B*** calculated by the singular value decomposition:

$$\boldsymbol{B} = (\boldsymbol{X}^{\tau}\boldsymbol{X})^{-1}\boldsymbol{X}^{\tau}\boldsymbol{Y}$$

where ***X*** and ***Y*** are the matrices of independent and dependent variables, respectively. Every possible regression model was built and thoroughly validated by the *leave-one-out cross-validation* technique (LOO-CV). Inspection of the models up to the *i*-th order for 1D, 2D and 3D models (with visualization) and higher dimensional *n*D models will be presented. Selection of the most optimal representations based on the adjusted and predicted R^2 values, LOO-CV mean squared error as well as the total number of variables in the model will be discussed.

REFERENCES

[1] T. Hrenar, ***moonee***, Code for Manipulation and Analysis of Multi- and Univariate Data, rev. 0.6826, 2021.

ANALYSIS OF DYNAMIC AND NONDYNAMIC CORRELATION DIAGNOSTICS

Xiang Xu,[a] Sebastian Sitkiewicz,[a] Eloy Ramos-Cordoba,[a] Xabier Lopez,[a] and Eduard Matito[a,b]

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A few years ago, our group has proposed new indices to quantify the importance of dynamic and nondynamic electron correlation in molecules. Namely, the dynamic and nondynamic indices I_D and I_{ND},[1] defined in terms of natural orbital occupancies, n_i^σ, have been suggested. More recently, Martin and coworkers[2] have reported comparisons among the T_1, D_1, and D_2 diagnostics (specific for coupled-cluster (CC) wavefunctions), the I_D and I_{ND} indices, and the von Neumann entropy S_{corr}, based on complete-basis-set-limit CCSD-F12 computations. They concluded that I_{ND} strongly correlates with von Neumann's entropy S_{corr}, both of them are not size-intensive, while the ratio $r_{ND} = \frac{I_{ND}}{I_D + I_{ND}}$ gives a similar performance to the T_1 diagnostic of CCSD.[2]

In this work, we propose the following normalization factor to solve the size-extensive problem,[2]

$$I_D = \sqrt{\frac{8}{M\ N}}\left(\frac{1}{4}\sum_{\sigma,i}\left[n_i^\sigma\left(1-n_i^\sigma\right)\right]^{1/2} - \frac{1}{2}\sum_{\sigma,i} n_i^\sigma\left(1-n_i^\sigma\right)\right) \quad (1)$$

$$I_{ND} = \frac{1}{N}\sum_{\sigma,i} n_i^\sigma\left(1-n_i^\sigma\right) \quad (2)$$

M being molecular orbital number and *N* the total electron number. We also analyze the performance of these new I_D and I_{ND} indices and over 20 other correlation diagnostics in a series of molecules using CCSD and CASSCF wavefunctions. Namely, we study hydrogen and polyacetylene chains [$(H_2)_n$ and C_nH_{n+2}] of different lengths, p-quinodimethane (PQM) upon elongation of the acetylene bonds and the twist of the acetylene bond in the C_2H_4 molecule. Both distortions are known to induce large nondynamic correlation effects. We find that T_1, D_1, and D_2 diagnostics correlate well with the largest occupation number in unoccupied natural orbitals (NON) which can be obtained in a cheaper way, while our indice I_{ND} correlates better with correlation entropies.

REFERENCES

[1] (a) E. Ramos-Cordoba, P. Salvador, E. Matito, *Phys. Chem. Chem. Phys.* 18 (2016), 24015–24023. (b) E. Ramos-Cordoba, E. Matito, *J. Chem. Theory Comput*. 13 (2017), 2705-2711, and references therein.
[2] M. Kesharwani, N. Sylvetsky, A. Köhn, D. P. Tew, J. M. Martin, *J. Chem. Phys.* 149 (2018), 154109

POSTSCRIPT ON VIABLE GROUND-STATES FOR CALCULATING TOPOLOGICAL π-ELECTRON RING-CURRENTS USING THE HÜCKEL–LONDON–POPLE–MCWEENY MODEL

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Attention is drawn to the idea that, in the context of the Hückel–London–Pople–McWeeny (HLPM) approach[1–4] to π-electron ring-currents, the basic *Aufbau* process[5,6] can be mimicked by means a graph-theoretical algorithm and that the outcome is determined solely by the *order* of the eigenvalues of the arbitrary molecular-graph representing an extant or hypothetical conjugated system. The *Aufbau* process usually results in a closed-shell ground-state, but sometimes a unique triplet ground-state arises,[7] sometimes doublets, as well as unique ground-states of higher multiplicity are encountered, and, on occasions, no uniquely defined π-electronic ground-state is established at all. Previously, the only examples of the latter ('pathological') case — which, as with triplet ground-states and other ground states that are not singlets, precludes the possibility of any HLPM calculation — were graphs that are unlikely candidates for being extant or viable conjugated systems.[8] In this note, however, an example is documented of what is, ostensibly, a plausible unsaturated structure — namely, $(\text{Coronene})^{6-}$. In the conclusion, attention is drawn to a procedure that averages electron distribution amongst the several orbitals of a degenerate shell.[9]

REFERENCES

[1] R. B. Mallion, *Croat. Chem. Acta* 81 (2008) 227–246.
[2] A. T. Balaban, T. K. Dickens, I. Gutman, & R. B. Mallion, *Croat. Chem. Acta* 83 (2010) 209–215.
[3] T. K. Dickens & R. B. Mallion, *Croat. Chem. Acta*, 86 (2013) 387–406.
[4] T. K. Dickens & R. B. Mallion, *MATCH Commun. Math. Comput. Chem.* 76 (2016) 297–356.
[5] F. A. Cotton, *Chemical Applications of Group Theory*, John Wiley & Sons, New York & London, 1963, pp 123–125
[6] C. A. Coulson, B. O'Leary, & R. B. Mallion, *Hückel Theory for Organic Chemists*, Academic Press, London, 1978.
[7] T. K. Dickens & R. B. Mallion, *Croat. Chem. Acta* 92 (2019) 445–455.
[8] R. B. Mallion & D. H. Rouvray, *Mol. Phys*. 36 (1978) 125–128.
[9] P. W. Fowler, W. Myrvold, C. Gibson, J. Clarke, & W. H. Bird, *J. Phys. Chem. A* 124 (2020) 4717–4533, especially p. 4528.

THE DERIVATION OF FORMULAS FOR CALCULATION OF CHARACTERISTIC VALUES OF STATISTICAL PARAMETERS USED IN MODEL QUALITY ESTIMATION

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Recently, a new accuracy parameter was introduced for binary classification models, that can be used for estimating the (real) model contribution which is over the level of random accuracy [1,2]. The randomization of the Y variable is used as a standard procedure in the model quality analysis in general, but particularly in the modelling of relationships between the structure and property/activity (QSP(A)R) of chemical compounds. A good result of randomization analyses for a model is when its actual accuracy, estimated by a selected statistical measure (parameter) of model quality, is significantly higher than the accuracy obtained by the best-randomized model. In binary classification models, both the experimental variable Y and corresponding model variable Y' (estimated/predicted by the model) have values of 0 or 1 (inactive/active). The values of each statistical measure (parameters, metrics) of such a model, derived from the comparison of experimental (Y) and model (Y') variables, can be expressed by four numbers forming a confusion matrix/table. These are TP (true positive) and TN (true negative) representing the total number of correct classification (when the same values are in variables Y and Y'), and FN (false negative) and FP (false positive) that are incorrect predictions. By performing permutation analysis of the values of model variable Y' keeping variable Y in the original order, we defined the characteristic values of the statistical measure (metric, parameter) as the border values (i.e. minimal and maximal) and the most probable (random) value. We derived the formulae for estimating the characteristic values of accuracy parameter (metric) measuring the percent of correct classification. Also, the usefulness of derived parameters will be illustrated in the analysis of the quality of balanced and non-balanced QSP(A)R models and confirmed by simulation results. Further, the possibility of application of the developed methodology in estimating the complexity of binary classification variables and models will be elaborated and generalized to multi-class problems.

ACKNOWLEDGEMENT

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REFERENCES

[1] J. Batista, D. Vikić-Topić, B. Lučić, *Croat. Chem. Acta* 89 (2016) 527–534.

[2] B. Lučić, J. Batista, V. Bojović, M. Lovrić, A. Sović Kržić, D. Bešlo, D. Nadramija, D. Vikić-Topić, *Croat. Chem. Acta* 92 (2019) 379–391.

POLYPHENOLS AS NATURAL SCAVENGERS OF CHEMICAL CARCINOGENS: A COMPUTATIONAL APPROACH

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Tannins are natural compounds that have historically been used in the tanning of leather. In the scientific literature, one finds many reports of their possible beneficial health effects, although these are not always unequivocally confirmed. In addition, [6]-gingerol from ginger has received considerable attention as a potential cancertherapeutic agent because of its chemopreventive and chemotherapeutic effects, as well as its safety. In the current study, we examined tannin basic building blocks and [6]-gingerol as natural scavengers of nine ultimate chemical carcinogens of the epoxy type to which we are frequently exposed: glycidamide, styrene oxide, aflatoxin B1 exo-8,9-epoxide, β-propiolactone, ethylene oxide, propylene oxide, 2-cyanoethylene oxide, chloroethylene oxide, and vinyl carbamate epoxide. To evaluate their efficacy, we expanded our research with the examination of glutathione – the strongest natural scavenger in human cells. The corresponding activation free energies were calculated using Hartree-Fock method with three flexible basis sets and two implicit solvation models. Epicatechin and [6]-gingerol represent natural compounds with the highest scavenging potential thus encouraging and guiding future experimental studies of their anticarcinogenic properties.

REFERENCES

[1] G. Hostnik, M. Gladović and U. Bren, *J. Nat. Prod.* 82 (2019) 3279−3287.
[2] V. Furlan and U. Bren, *Int. J. Mol. Sci.* 21 (2020) 695.

RANDIĆ CONNECTIVITY INDEX AND ITS VARIATIONS FOR QSPR MODELLING OF AQUEOUS SOLUBILITY

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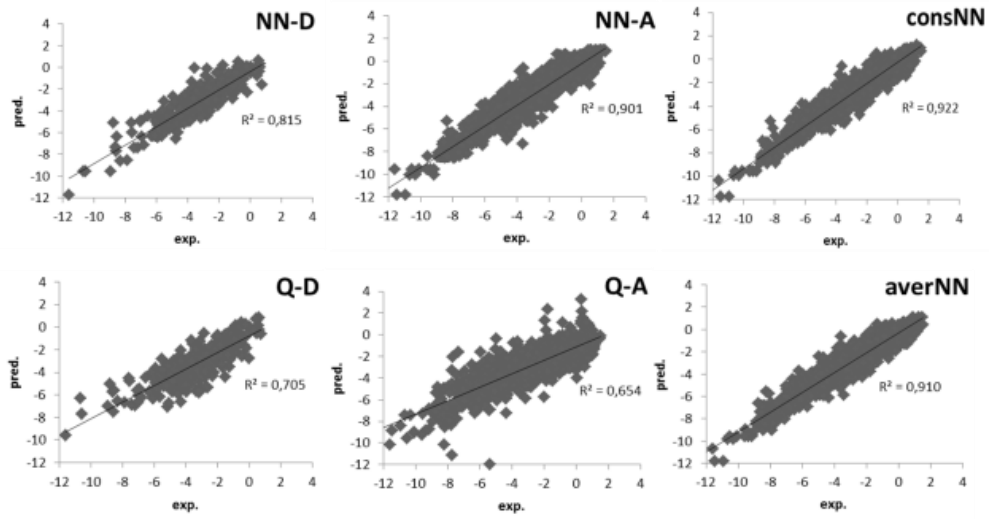
QSPR (quantitative structure-property relationship) models were developed to predict aqueous solubility (log S). The dataset for training or optimize the neural network or linear models were taken from the AqSolDB database and consisted of over 1600 compounds with experimentally determined solubility values. Structural descriptors, including the Randić connectivity index [1] were used to represent chemical structure of molecules from the dataset. We have compared the models based on Randić-like indices with those from AqSolDB database [2]. The models were validated with external prediction sets, with the root mean squared errors (RMSE) ranging from 0.8 to 1.1 log units. Interestingly, the RMSE of models based on the Randić-like descriptors only, were in average only 0.2 log units larger than the models with 17 preselected as suitable descriptors for modelling aqueous solubility.



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REFERENCES

[1] M. Randić, *J. Am. Chem. Soc*. **1975**, *97*(23), 6609.
[2] M. C. Sorkun, A. Khetan, S. Er, *Sci Data*. **2019**, *6*(143). https://doi.org/10.1038/s41597-019-0151-1.

SPECTRAL EXTREMAL TREES WITH DEGREE-BASED WEIGHTS

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In recent years, many weighted adjacency matrices from graphs weighted by degree-based indices have been proposed and studied, such as Randic matrix, ABC matrix, AG matrix, etc. For each of them one needs to study its spectral properties, especially spectral radius and the corresponding extremal graphs. However, the used methods look very similar. A natural question is how can we work out a unified method to deal with the spectral problem for these seemingly different kinds of weighted adjacency matrices. This talk will show you a first try to address this question for the spectral extremal trees with degree-based weights.

EFFICIENT APPLICATION OF MODULAR GRAPH TRANSFORMATION RULES

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Graph transformation formalisms have proven to be suitable tools for the modeling of chemical reactions. They are well established in theoretical studies [3] and increasingly also in practical applications to chemistry [2,4]. The latter is made feasible via the establishment of programming frameworks which make the formalisms executable [1].

The application to large networks of chemical reactions, however, poses unique computational challenges. One prominent characteristic of this application is the inherent modularity of the graphs involved, as these graphs are composed of many connected components each representing a molecule. While the existing methods for implementing graph transformations formally can be applied to such disconnected graphs, the graph isomorphism checking parts of the methods quickly become the computational bottleneck when the size of the chemical reaction network grows.

In this article, we develop a new method of applying graph transformation rules, which can speed up applications such as these. The method is based on reducing the graph isomorphism checking problem to smaller instances by utilizing the knowledge of different connected components and working on the graph in a piece-wise fashion. We further extend the algorithm with an efficient heuristic, based on local symmetries of the graphs, for pruning partial applications to only enumerate derivations unique up to isomorphism. Finally, we conduct various chemical network generation experiments on real life as well as synthetic data and compare against state-of-the-art in the field.

REFERENCES

[1] J. L. Andersen, C. Flamm, D. Merkle, and P. F. Stadler. A software package for chemically inspired graph transformation. In *International Conference on Graph Transformation*, pp. 73–88. Springer, 2016.

[2] G. Benkö, C. Flamm, and P. F. Stadler. A graph-based toy model of chemistry. *Journal of Chemical Information and Computer Sciences*, 43(4):1085–1093, 2003.

[3] U. P. G Taentzer and H. E. K Ehrig. Fundamentals of algebraic graph transformation. with 41 figures (monographs in theoretical computer science. an eatcs series), 2006.

[4] M. K. Yadav, B. P. Kelley, and S. M. Silverman. The potential of a chemical graph transformation system. In *International Conference on Graph Transformation*, pp. 83–95. Springer, 2004.

MAYGEN - AN OPEN-SOURCE CHEMICAL GRAPH GENERATOR BASED ON THE ORDERLY GENERATION PRINCIPLE

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The generation of chemical graphs has been a subject of cheminformatics since the early 1960s. To perform such a generation isomorphism-free, the structure generator needs to ensure the building of canonical graphs already during the generation step and not by subsequent filtering. Here we present MAYGEN [1] an open-source, pure-Java development of a chemical graph generator based on the orderly generation principle. MAYGEN is benchmarked against the state-of-the-art, but closed-source solution MOLGEN [2], as well as against the best open-source solution OMG [3]. MAYGEN outperforms OMG by an order of magnitude and gets close to MOLGEN in performance (Figure 1).

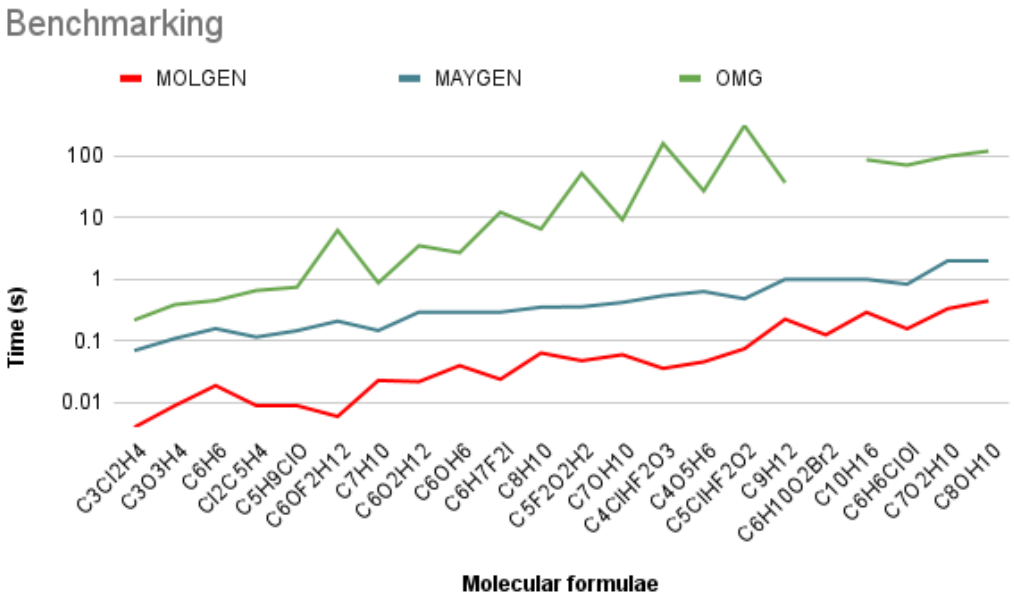

Figure 1. Benchmarking of MOLGEN, MAYGEN and OMG with molecular formulae containing carbon, hydrogen, oxygen, and halogens.

REFERENCES

[1] Yirik MA, Sorokina M, Steinbeck C. MAYGEN-an Open-Source Chemical Structure Generator for Constitutional Isomers Based on the Orderly Generation Principle.

[2] Gugisch R, Kerber A, Kohnert A, Laue R, Meringer M, Rücker C, Wassermann A. MOLGEN 5.0, a molecular structure generator. InAdvances in mathematical chemistry and applications 2015 Jan 1 (pp. 113-138). Bentham Science Publishers.

[3] Gugisch R, Kerber A, Kohnert A, Laue R, Meringer M, Rücker C, Wassermann A. MOLGEN 5.0, a molecular structure generator. InAdvances in mathematical chemistry and applications 2015 Jan 1 (pp. 113-138). Bentham Science Publishers.

ON MARGINAL ENTROPY OF GRAPHS

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The first entropy measure was defined by Shannon in 1948 [1]. Bonchev and Trinajstic introduced an entropy measure which is based on distances to interpret the molecular branching of molecular graphs [2]. Later they applied the information theory in characterization of chemical structures [3,4]. These molecular descriptors were called information indices and it was shown that the information indices have greater discriminating power for molecules than the respective topological indices [5]. Marginal entropy was defined by Konstantinova [5] which is based on distance of vertices. Wiener index was defined in 1947 and it equals to one half of total distances between every pair of vertices in a graph [6]. The marginal entropy of a graph G was defined by the following equation

$$I_D(G) = -\sum_{u \in V(G)} \frac{D(u)}{2W(G)} \log\left(\frac{D(u)}{2W(G)}\right)$$

such that $D(u)$ denotes the total distance of a vertex $u \in V(G)$. In this paper we calculate the marginal entropy of some graphs and investigate properties of this entropy.

REFERENCES

[1] C. Shannon, W. Weaver, *University of Illinois*, Urbana, 1949.
[2] D. Bonchev, N. Trinajstic, *J. Chem. Phys.* 38 (1977) 4517–4533.
[3] D. Bonchev, N. Trinajstic, *Int. J. Quantum Chem*. 12 (1978) 293–303.
[4] D. Bonchev, N. Trinajstic, *Intern. J. Quantum Chem. Symp.*16 (1982) 463-480.
[5] E.V. Konstantinova, *J. Chem. Inf. Comput. Sci.* 36 (1996) 54–57.
[6] A. H. Wiener, *J. Am. Chem. Soc*. 69 (1947) 17-20.

TREES WITH EXTREMAL GRAOVAC-GHORBANI INDICES

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Let $G=(V,E)$ be a simple undirected and connected graph of order *n*. In 2010. Graovac and Ghorbani introduced a distance-based analog of the well-known atom-bond connectivity index, nowadays known as the Graovac-Ghorbani index. It is defined as

$$GG(G)=\sum_{uv\in E}\sqrt{\frac{n_u+n_v-2}{n_u n_v}},$$

where n_u is the number of vertices of *G* lying closer to *u* than to *v* and n_v is the number of vertices of *G* lying closer to *v* than to *u*. In this paper we consider *n*-vertex trees with bounder maximum degree and those with prescribed degree sequence and find the ones that have extremal *GG* indices.

REFERENCES

[1] D. Dimitrov, B. Ikica, R. Škrekovski, Remarks on the Graovac-Ghorbani Index of Bipartite Graphs, *Applied Mathematics and Computations* 293 (2017), 370–376.

ON *VE*-DEGREE IRREGULARITY INDICES OF SOME MOLECULAR STRUCTURES

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Domination is one of the most important graph invariants. It has been shown that domination is a very sensitive graph theoretical invariant to even the slightest changes in a graph [1]. Domination was studied for chemical materials in the past. For example, the domination number of benzenoid chains and hexagonal grid was obtained by Vukicevic and Klobucar [1]. Vertex-edge domination is one of the mixed type domination invariants. A vertex *v* dominates an edge *e* which is incident to *v* or incident to a neighbor of *v*. Therefore, *ve*-degree of a vertex *v* equals to number of different edges which are incident to a vertex from the closed neighborhood of [2]. Total number of *ve*-degrees of vertices equals to First Zagreb Index for tri-angle free graphs [2]. The *ve*-degree concept has been successfully applied to Chemical Graph Theory [3]. More than forty papers have been written on this topic. It has been shown that *ve*-degree topological indices can be used as possible tools in QSPR researches. Albertson index is one of the irregularity indices [4]. It has been called as Third Zagreb Index. In this paper, we study *ve*-degree Albertson index, *ve*-degree total irregularity index and *ve*-degree variance of some molecular structures.

REFERENCES

[1] D.Vukicevic, A. Klobucar, *Croatica Chemica Acta* 80 (2) (2007) 187-191.
[2] M. Chellali, T. W. Haynes, S. T. Hedetniemi, T. M. Lewis, *Discrete Mathematics* 340 (2017) 31−38.
[3] B. Sahin, S. Ediz, *Iranian J. Math Chem*. 9 (4) 263-277.
[4] M. O. Albertson, *Ars Combin*. 46 (1997), 219-225.

CONTRIBUTION OF C-RING HYDROGENS TO FREE RADICAL SCAVENGING BY EQUOL

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Epidemiological studies have shown that diets rich in soy isoflavones are beneficial to human health [1]. However, these benefits aren't ascribed to parental molecules of ingested isoflavones but to their intestinal metabolites [2]. Among these metabolites, equol has been extensively studied because of its bioactivity [3,4], which may help to reduce the incidence of age-related disorders [1]. In this work, free radical scavenging potency of equol was investigated by using M06-2X/6-311++G(d,p) level of theory, accompanied with the TST and Eckart tunneling corrections for the estimation of rate constants. The influence of solvents was calculated with an implicit continuum solvation model, SMD [5]. Spin unrestricted calculations were used for open-shell systems. Local minima and transition states (TSs) were identified by the number of imaginary frequencies (0 and 1, respectively). Intrinsic reaction coordinate calculation was performed on both sides of the TS to confirm that it properly connects with the corresponding reactants and products. All computations were performed in gas-phase, pentyl ethanoate and water at 298.15 K. BDE related to H-atom donation was calculated as described elsewhere [6]. Performed electronic structure and kinetic calculations indicate phenolic hydrogens of equol as much more abstractable than C-ring hydrogens. Thus, the C-ring hydrogens are poor HOO• scavengers with negligible contribution to equol antioxidant potency. This is in line with the known facts related to phenolic O−H vs C−H reactivity and structural requirements needed for antioxidant activity of flavonoids, but opposite to recently published predictions.

REFERENCES

[1] B. Mayo, L. Vazquez, A.B. Florez, *Nutrients* 11 (2019) 2231.
[2] B.-J. Li, *J. Food Process. Preserv.* 43 (2019) e14205.
[3] C.E. Rüfer, S.E. Kulling, *J. Agric. Food. Chem*. 54 (2006) 2926-2931.
[4] K.D.R. Setchell, C. Clerici, E.D. Lephart, S.J. Cole, C. Heenan, D. Castellani, B.E. Wolfe, *Am. J. Clin. Nutr*. 81 (2005) 1072-1079.
[5] A.V. Marenich, C.J. Cramer, D.G. Truhlar, *J. Phys. Chem. B* 113 (2009) 6378-6396.
[6] A. Amić, B. Lučić, V. Stepanić, Z. Marković, S. Marković, J.M. Dimitrić Marković, D. Amić, *Food Chem*. 218 (2017) 144-151.

MULTI-TARGET ANTIMICROBIAL ACTIVITY MODEL OF *CINCHONA* ALKALOIDS ESTABLISHED BY MACHINE LEARNING

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Antimicrobial activity of *Cinchona* alkaloids derivatives [1] was previously evaluated by using disc diffusion assay against a panel of various Gram-positive and Gram-negative bacteria. Principal components of the activity data were extracted by 2nd-order tensor decomposition and used as dependent variables for multivariate linear regression, whereas theoretically computed energy fingerprints of all compounds were used as independent variables. Potential energy surfaces (PES) of compounds were sampled by performing molecular dynamics simulations and then decomposed by principal component analysis.

Regression models were generated by extensive machine learning multivariate linear regression – linear combinations of original variables were used as well as their higher-order polynomial terms. Obtained models were thoroughly validated by *leave-one-out cross-validation* technique (LOO-CV) [2]. The optimal activity/PES model based on the adjusted and the predicted R^2 values as well as LOO-CV mean squared error will be presented.

REFERENCES

[1] A. Bosak, A. Ramić, T. Šmidlehner, T. Hrenar, I. Primožič, Z. Kovarik, *PLoS ONE* **13**(10): e0205193.
[2] T. Hrenar, ***moonee***, Code for Manipulation and Analysis of Multi- and Univariate Data, rev. 0.6826, 2021.

INHIBITORY ZINC ION BINDING SITE AND THE METAL EXCHANGE MECHANISM IN HUMAN DPP III

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DPP III is the only metalloenzyme among the dipeptidyl peptidases. It is ubiquitously present in organisms ranging from bacteria to humans and is found in almost all human tissues.[1] In addition to its role in the final stages of protein turnover, it is also involved in blood pressure regulation,[2] oxidative stress response[3] and because of its affinity and activity toward neuropeptides,[4] it is thought to be involved in pain regulation. Experimental data indicates the possible importance of DPP III in cancer. In addition, recent studies have shown that DPP III is a biomarker candidate for the severity of cardiac shock and a potential target for heart failure therapy.[5] The importance of DPP III in human health, combined with the experimental finding that excess zinc inhibits its hydrolytic activity, prompted us to investigate the binding of the second zinc ion into the active site of human DPP III and its influence on enzyme structure and dynamics. Using QMMM calculations in combination with the comprehensive MD simulations, we investigated several di-metal structures of the ligand-free enzyme as well as the DPP III -hemorfin-like peptide-IVYPW complex. The obtained results revealed the position and structure of the binding site for the inhibitory zinc ion in DPP III. Moreover, the metal exchange pathway was traced, indicating an associative type of metal exchange in DPP III.

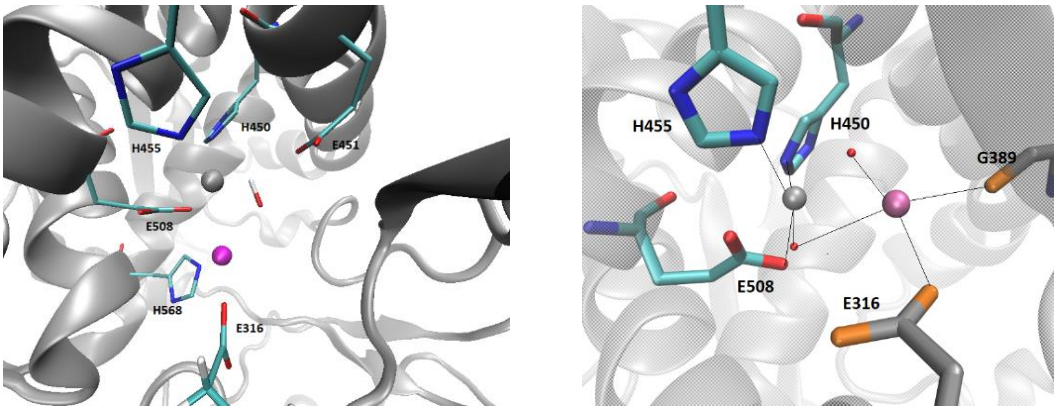

Figure 1. Two common binding modes of zinc ion into the DPP III interdomaun cleft. The catalytically active Zn is colored gray, and the second, inhibitory Zn, magenta. Water molecules are shown as small red spheres.

REFERENCES

[1] S. Abramić, Marija, Gruber, K., Macheroux, P., Tomić, in Handbook of Proteolytic Enzymes: Metallopeptidases, ed. N. D. Rawlings & D. S. Auld, Elsevier, San Diego, 4th edn., 2022.

[2] S. Jha, U. Taschler, O. Domenig, M. Poglitsch, B. Bourgeois, M. Pollheimer, L. M. Pusch, G. Malovan, S. Frank, T. Madl, K. Gruber, R. Zimmermann and P. Macheroux, *J. Biol. Chem.* 295 (2020) 13711–13723.

[3] B. E. Hast, D. Goldfarb, K. M. Mulvaney, M. A. Hast, P. F. Siesser, F. Yan, D. N. Hayes and M. B. Major, *Cancer Res*. 73 (2013) 2199–221.

[4] A. Tomić, B. Kovačević and S. Tomić, *Phys. Chem. Chem. Phys*. 18 (2016) 27245–27256.

[5] A. Magliocca, T Omland and R. Latini, *Eur. J. Heart Fail.* 22 (2020) 300–302.

NIDO CAGE···π NON-COVALENT INTERACTIONS

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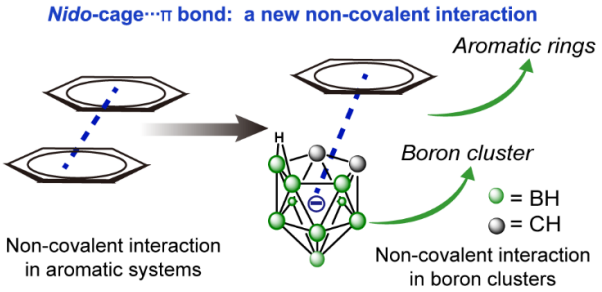
In the first part of the lecture, we will discuss the aromaticity of *closo* and *nido* boranes [1]. Then, we will report a new type of non-covalent interaction, *nido*-cage···π bond, between the boron cluster $C_2B_9H_{12}^-$ and an aromatic π system [2]. The X-ray diffraction studies indicate that the *nido*-cage···π bonding presents the same parallel-displaced or T-shaped geometries as a π···π interaction does [3]. The contacting distance between the cage and the π ring varies with the type and the substituent of the aromatic ring. Quantum chemical calculations reveal that, first, the *nido* cage retain part of the aromatic character that characterizes the *closo* borane cages [1], and, second, this *nido*-cage···π non-covalent interaction shares a similar nature to the conventional anion···π [4] or π···π [3] bond found in classical aromatic ring systems. Our theoretical calculations reveal a major electrostatic character or orbital- and dispersion-dominated interaction, similar to those found in cyclopentadienyl anion···π or π···π interactions.



REFERENCES

[1] J. Poater, M.; C. Viñas, M. Solà and F. Teixidor, *J. Am. Chem. Soc.* 142 (2020) 9396–9407.
[2] D. Tu, H. Yan, J. Poater, and M. Solà, *Angew. Chem. Int. Ed.* 59 (2020) 9018–9025.
[3] a) S. Tsuzuki, K. Honda, T. Uchimaru, M. Mikami and K. Tanabe, *J. Am. Chem. Soc.* 124 (2002) 104-112. b) M. Sinnokrot, E. F. Valeev and C. D. Sherrill, *J. Am. Chem. Soc.* 124 (2002) 10887-10893.
[4] a) D. X. Wang and M. X. Wang, *J. Am. Chem. Soc.* 135 (2013) 892-897. b) H. Liu, Q. Zhang and M. X. Wang, *Angew. Chem. Int. Ed.* 57 (2018) 6536-6540.

Mer-COORDINATION OF A MIXED IMINOACETAMIDE / (2-PICOYL)AMINE LIGAND TO THE Zn^{2+} CATION: X-RAY AND NMR STUDY

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In our research of iminodiacetamide (imda) [1] and bis(2-picolyl)amine (bpa) [2] ligands and their coordination to metal cations, we concluded that imda ligands form almost exclusively *trans-fac*, while bpa ligands gave preferentially *cis-fac* ML_2 isomers. Due to the inherent C_2 symmetry of *cis-fac* or *mer* ML_2 isomers, they are more interesting for potential usage in enantioselective catalysis. By preparation of the mixed imda-bpa tridendate ligand we aimed to increase the probability of metal complexation towards the C_2 symmetric structures.

Herein we present the preparation and NMR characterization of the mixed iPr-imda-bpa ligand L and its C_2 symmetric *mer*-$[ZnL_2]^{2+}$ complex. ^1H and ^{13}C NMR spectra of the ligand and complex in acetonitrile will be compared with theoretical DFT calculations based on a recently proposed scheme, [3] which consists of the exploration of conformer/ rotamer space by the CREST algorithm [4] and calculations of the free energies and Boltzmann populations by the ENSO utility. [3] Calculation of NMR parameters is performed by the ORCA program. [5] Additionally, we present a solid-state structure of the *mer* $[ZnL_2]^{2+}$ complex obtained by single-crystal X-ray diffraction. Single crystals are prepared by complexation of the ligand L with $Zn(BF_4)_2 \cdot \times H_2O$. The crystal structure includes the SiF_6^{2-} anions as a result of the decomposition of BF_4^- anions and reaction of the formed F^- anions with the glass vessel. [1] Obtained crystals of $2[ZnL_2][SiF_6][BF_4]_2 \times 8.5H_2O$ solvate crystallize in the highly symmetric cubic space group $Pn\bar{3}n$ (Nr. 222, a = 37.10182(10) Å) with 48 *mer* $[ZnL_2]^{2+}$ cations in the unit cell.

REFERENCES

[1] N. Pantalon Juraj, G. I. Miletić, B. Perić, Z. Popović, N. Smrečki, R. Vianello, S. I. Kirin, *Inorg. Chem.* **58** (2019) 16445–16457.
[2] N. Pantalon Juraj, S. Muratović, B. Perić, N. Šijaković Vujičić, R. Vianello, D. Žilić, Z. Jagličić, S. I. Kirin, *Cryst. Growth Des.* **20** (2020) 2440–2453.
[3] S. Grimme, C. Bannwarth, S. Dohm, A. Hansen, J. Pisarek, P. Pracht, J. Seibert, F. Neese, *Angew. Chem. Int. Ed*. **56** (2017) 12485–12491.
[4] P. Pracht, F. Bohle, S. Grimme, *Phys. Chem. Chem. Phys.* **22** (2020) 7169–7192.
[5] F. Neese, *Wiley Interdiscip. Rev.: Comput. Mol. Sci* **8** (2018) e1327.

WORKSHOP

MODELLING REACTIONS AT METAL-ORGANIC INTERFACES

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The modelling of organic chemical reactions on surfaces is a rapidly developing field bridging solid-state physics and chemistry. The use of surfaces opens up possibilities for chemically unusual reaction mechanisms and interesting (adsorbed) product structures, thus giving us new tools for both synthesis[1] and catalysis.[2,3]

In this workshop, a practical introduction to the capabilities of the the *Vienna Ab initio Simulation Package* (VASP) will be given. A variety of topics will be covered, highlighting differences between planewave-based software and programs more commonly used by chemists (*Turbomole*, *Gaussian*, *Orca*…). In the first part of the workshop, we will look at algorithms for structure relaxation and their typical issues (balancing electronic and ionic steps, accounting for Pulay stress, etc.). In the second part, we will focus on the calculation of properties in solids (e.g. IR and electronic spectra) and look at methods commonly used for finding transition states (nudged elastic band, following unstable vibrational modes). Finally, a short tutorial on running VASP using HPC resources will be given.

REFERENCES

[1] Clair, S.; de Oteyza, D.G. *Chem. Rev.* **2019**, *119* (7), 4717-4776.
[2] Bocque, M.; Loffreda D. J. Am. Chem. Soc. **2005**, 127 (49),17207-17215.
[3] Zaera, F. *ACS Catal*. **2017**, 7 (8), 4947-4967.

POSTERS

MODELLING PROTEIN FOLDING RATES BY NOVEL DESCRIPTORS BASED ON THE AMOUNT OF REGULAR SECONDARY STRUCTURE AND HYDROPHOBIC AMINO ACIDS

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Protein folding is a very important problem in the biosciences that is studied experimentally but also by modelling (theoretical and simulation analyses) [1]. Undoubtedly, all information related to folding is contained in the primary structure of proteins - in the sequence of amino acids. For the past 20 years, attempts have been made to model the dependences of the protein folding constants k_f (s^{-1}), which are equal to 1 / (time needed for protein folding). It was observed in the very beginning that this is a size-dependent problem, which means that ln(k_f) significantly depends on the length of the protein sequence, *i.e.* on the number of amino acid residues in the protein chain. Then, the dependence on the number of amino acids that take on the correct secondary structure of alpha or beta, on the topology of the 3D structure, was also observed [2].

As better predictors of protein folding constants, new structural parameters based on the total number of amino acids in regular secondary structures and on particular hydrophobic amino acids in the protein chain were obtained [3]. Furthermore, the parameters that calculate the permutation entropy of the secondary structure of the protein also show good agreement with the protein folding constants. In addition, the problem of experimental error in measuring protein folding constants was analyzed, as well as the problem of insufficiently given primary protein structures in research studies, and their influence on the final accuracy that can be expected in modelling protein folding constants.

ACKNOWLEDGEMENT:
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REFERENCES

[1] D. N. Ivankov, A. V. Finkelstein, Solution of Levinthal's paradox and a physical theory of protein folding times. *Biomolecules* 10 (2020) 250.
[2] S. Lifson, C. Sander C. Antiparallel and parallel beta-strands differ in amino acid residue preferences. *Nature* 282 (1979) 109–111.
[3] M. Levitt, Conformational preferences of amino acids in globular proteins. *Biochemistry* 17 (1978) 4277–4285.

TUNING THE OPTOELECTRONIC PROPERTIES OF DINITROSOARENE POLYMERS

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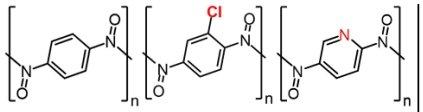
Organic semiconductors have been a subject of immense interest due to the possibility of their integration in electronic and optical devices such as photovoltaic diodes, polymer transistor circuits and light-emitting transistors.[1,2,3] However, finding suitable candidates within this broad class of materials is an ongoing challenge. It was recently shown that dinitrosobenzene may be used as an easily polymerizable molecular wire with the possibility of ON/OFF switching.[4]

Focusing on first principles calculations, we investigate how the electronic and optical properties of dinitrosoarene polymers can be tuned by chemical (by changing substituents or the aromatic core) or physical (adsorption on metal surfaces) modulation. Introducing either electron withdrawing or electron donating groups widens the band gap, which can be explained by a decrease in conjugation due to the increased torsional angle between the phenyl and azodioxy planes. Substituting the benzene ring with an aromatic heterocycle or a polycyclic arene shrinks the gap, also resulting in a strong decrease of electron mobility in the former case. Adsorbing the dinitrosobenzene polymer on a (111) gold surface induces the planarization of the polymer, which maximizes the conjugation along the polymer chain. This drastically lowers the bandgap. Further investigation of optical properties of these compounds by ellipsometry and AFM/STM is in progress.



HSE06	E_g [eV]	$m_{e,HOMO}$	$m_{e,LUMO}$
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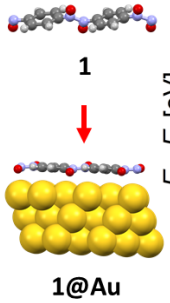
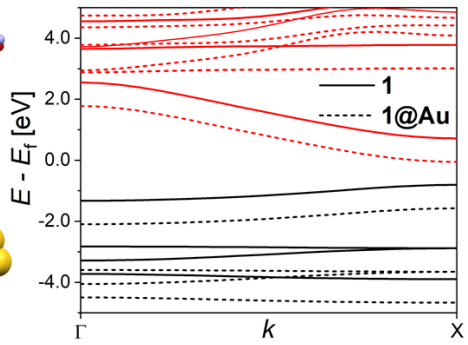
2	2.7	2.42	0.74
3	2.1	0.94	0.21





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REFERENCES

[1] O. Ostroverkhova, *Chem. Rev*. 116 (2016) 13279–13412.
[2] P. Thaneshwor, P. Kalonil, G. Schreckenbachl, M. S. Freund, *Sci. Rep*. 6 (2016) 36554–36572.
[3] D. Yuan, M. A. Awais, V. Sharapov, X. Liu, A. Neshchadin, W. Chen, L. Yu. *J. Am. Chem. Soc*. 143 (2021) 5239–5246.
[4] G. Gallo, A. Mihanović, I. Rončević, R. Dinnebier, H. Vančik, *Polymer* 214 (2021) 123235.

UNDERSTANDING THE HUMAN DPP III SUBSTRATE SPECIFICITY - QM/MM AND MD CALCULATIONS

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Dipeptidyl-peptidase III (DPP III; EC 3.4.14.4) is a two-domain monozinc exopeptidase of the peptidase family M49 that hydrolyzes dipeptides from the unsubstituted N-terminus of its substrates. Studies showed that tetrapeptides to octapeptides are the best substrates.[1,5] Although assumed to be an enzyme with broad substrate specificity[1,3-5] the exact kinetic parameters have been determined for only a few peptide substrates, such as: angiotensins,[4,5] proctolin,[6] α-melanocyte-stimulating hormone,[4] dynorphin A(1-8),[7] enkephalins[3] and endomorphins,[7] as well as some hemorphins[7] and exorphins.[7] All these findings suggest that DPP III may play physiological role in regulating the disposition of bioactive peptides. At the same time tynorphin (VVYPW), the truncated form of spinorphin, showed inhibitory activity toward DPP III isolated from monkey brain.[8,9] Chiba *et al.* examined the inhibitory activities of various synthetic hemorphin-like peptides and found that the tynorphin analogs IVYPW and WVYPW showed even stronger inhibitory activity toward rat DPP III.[11] Kumar *et al.* characterized tynorphin as a weak substrate of DPP III.[11] One of the possible reasons why DPP III cleaves peptides with different sequences and sizes is its flexibility and thus adaptability of its binding site to accommodate molecules of different sizes. To better understand DPP III substrate specificity, we have investigated the catalytic performance of the enzyme in tynorphin hydrolysis by quantum mechanical – molecular mechanical calculations and molecular dynamics simulations, using the previously determined mechanism of hydrolysis in the DPP III – Leu-enkephalin complex as a starting point for these studies.[12]

REFERENCES

[1] S. Ellis, J. M. Nuenke, *J. Biol. Chem.* **1967**, *242* (20), 4623–4629.
[2] S. Simaga, D. Babić, M. Osmak, M. Sprem, M. Abramić, *Gynecol. Oncol.* **2003**, *91* (1), 194–200.
[3] C. M. Lee, S. H. Snyder, *J. Biol. Chem.* **1982**, *257* (20), 12043–12050.
[4] M. Abramić, M. Zubanović, L. Vitale, *Biol. Chem. Hoppe. Seyler.* **1988**, *369* (1), 29–38.
[5] M. Smyth, G. O'Cuinn, *J Neurochem.* **1994**, *63* (4), 1439–1445.
[6] C. Mazzocco, J. Gillibert-Duplantier, V. Neaud, K. M. Fukasawa, S. Claverol, M. Bonneu, J. Puiroux, *FEBS J.* **2006**, *273* (5), 1056–1064.
[7] M. Barsun, N. Jajcanin, B. Vukelić, J. Spoljarić, M. Abramić, *Biol. Chem.* **2007**, *388* (3), 343–348.
[8] K. Nishimura, T. Hazato, *Biochem. Biophys. Res. Commun.* **1993**, *194* (2), 713–719.
[9] Y. Yamamoto, J. Hashimoto, M. Shimamura, T. Yamaguchi, T. Hazato, *Peptides* **2000**, *21* (4), 503–508.
[10] T. Chiba, Y.-H. Li, T. Yamane, O. Ogikubo, M. Fukuoka, R. Arai, S. Takahashi, T. Ohtsuka, I. Ohkubo, N. Matsui, *Peptides* **2003**, *24* (5), 773–778.
[11] P. Kumar, V. Reithofer, M. Reisinger, S. Wallner, T. Pavkov-Keller, P. Macheroux, K. Gruber, *Sci. Rep.* **2016**, *6*, 23787.
[12] A. Tomić, B. Kovačević, S. Tomić, Phys. Chem. Chem. Phys. 2016, 18 (39), 27245–27256.

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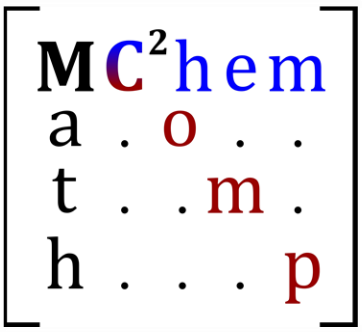

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