

Riešiteľ	DUBECKÝ Matúš
Pozícia na projekte	Vedecko-výskumný pracovník
Vedecké identifikátory	WoS (Researcher ID): P-1720-2016, Scopus (AuthorID): 56358387500, ORCID: 0000-0002-3975-1106
Vedecké zameranie	počítačové modelovania elektrónovej štruktúry komplexných materiálov z prvých princípov (kvantové Monte Carlo)
Publikačná činnosť s ohlasmí (aktuálne k 31.10.2022)	
V3 Vedecký výstup publikačnej činnosti z časopisu	
V3_01	DITTE, Matej - DUBECKÝ, Matúš. Fractional charge by fixed-node diffusion Monte Carlo method. In <i>Physical Review Letters</i> . Vol. 123, (2019), s. 1-6. ISSN 0031-9007 (2019: 8.385 - IF, Q1 - JCR Best Q, 3.588 - SJR, Q1 - SJR Best Q). V databáze: DOI: 10.1103/PhysRevLett.123.156402 ; WOS: 000489255900008 ; CC: 000489255900008 ; SCOPUS: 2-s2.0-85073445890. Kategória publikácie do 2021: ADC
V3_02	DUBECKÝ, František - DUBECKÝ, Matúš - HUBÍK, Pavel - KINDL, D. - GOMBIA, Enos - BALDINI, M. - NEČAS, Vladimír. Unexpected Current Lowering by a Low Work-Function Metal Contact: Mg/Si-GaAs. In <i>Solid-State Electronics</i> . Vol. 82 (2013), s.72-76. ISSN 0038-1101 (2013: 1.514 - IF, Q2 - JCR Best Q, 0.770 - SJR, Q1 - SJR Best Q). Kategória publikácie do 2021: ADC Ohlasy: 1. [1] CHEN, Bingbing - CHEN, Jianhui - SHEN, Yanjiao - GE, Kunpeng - GUO, Jianxin - LI, Feng - LIU, Haixu - XU, Ying - MAI, Yaohua. Magnesium thin film as a doping-free back surface field layer for hybrid solar cells. In <i>APPLIED PHYSICS LETTERS</i> , 2017, vol. 110, no. 13, pp. ISSN 0003-6951., Registrované v: WOS, SCOPUS Ohlas: zahraničný 2. [1] CHERNYKH, S. V. - CHERNYKH, A. V. - CHUBENKO, A. P. - PAVLYUCHENKO, L. N. - SVESHNIKOV, Yu. N. - GLYBIN, Yu. N. - KONOVALOV, M. P. - PANICHKIN, A. V. - DIDENKO, S. I. Detectors on the Basis of High-Purity Epitaxial GaAs Layers for Spectrometry of X and Gamma Rays. In <i>INSTRUMENTS AND EXPERIMENTAL TECHNIQUES</i> , 2018, vol. 61, no. 5, pp. 665-672. ISSN 0020-4412., Registrované v: WOS, CC, SCOPUS Ohlas: zahraničný 3. [1] JIANG, Haiyan - YANG, Xueliang - WEN, Zhixi - GE, Kunpeng - LI, Feng - CHEN, Jingwei - XU, Ying - SONG, Dengyuan - CHEN, Jianhui. Considerably Improved Photovoltaic Performances of ITO/Si Heterojunction Solar Cells by Incorporating Hydrogen into Near-Interface Region. In: <i>IEEE Journal of Photovoltaics</i> , 2022-09-01, 12, 5, pp. 1102-1108. ISSN 21563381., Registrované v: SCOPUS, WOS, CC Ohlas: zahraničný
V3_03	DUBECKÝ, František - OSWALD, Jiří - KINDL, Dobroslav - HUBÍK, Pavel - DUBECKÝ, Matúš - GOMBIA, Enos - ŠAGÁTOVÁ, Andrea - BOHÁČEK, Pavol - SEKÁČOVÁ, Mária - NEČAS, Vladimír. Photocurrent spectra of semi-insulating GaAs M-S-M diodes: Role of the contacts. In <i>Solid-State Electronics</i> . Vol. 118, (2016), s. 30-35. ISSN 0038-1101 (2016: 1.580 - IF, Q3 - JCR Best Q, 0.544 - SJR, Q2 - SJR Best Q). V databáze: CC: 000369831300006. Kategória publikácie do 2021: ADC Ohlasy: 1. [1] ABDULKHAEV, Oybek - YAKUBOV, Anvar - GIYASOVA, Feruza - KHAKIMOV, Alim - YODGOROVA, Dilbara - KARIMOV, Abdulaziz. Electrical properties and photosensitivity of multi-barrier photodiode structure based on semi-insulating gaas. In <i>2020 International Conference on Information Science and Communications Technologies, ICISCT 2020, 2020-11-04</i> , pp., Registrované v: SCOPUS Ohlas: zahraničný
V3_04	DUBECKÝ, František - ZAŤKO, Bohumír - KOLESÁR, Vladimír - KINDL, D. - HUBÍK, Pavel - GOMBIA, Enos - DUBECKÝ, Matúš. Charge collection efficiency of Pt vs. Mg contacts on semi-insulating GaAs. In <i>Applied Surface Science</i> . Vol. 467-468, (2019), s. 1219-1225. ISSN 0169-4332 (2019: 6.182 - IF, Q1 - JCR Best Q, 1.230 - SJR, Q1 - SJR Best Q). V databáze: SCOPUS: 2-s2.0-85056169728 ; DOI: 10.1016/j.apsusc.2018.10.164 ; CC: 000451023500139 ; WOS: 000451023500139. Kategória publikácie do 2021: ADC
V3_05	DUBECKÝ, Matúš. Bias cancellation in one-determinant fixed-node diffusion Monte Carlo: Insights from fermionic occupation numbers. In <i>Physical Review E</i> . Vol. 95, iss. 3 (2017), s. 033308-1 - 033308-7. ISSN 2470-0045 (2017: 2.284 - IF, Q1 - JCR Best Q, 0.979 - SJR, Q1 - SJR Best Q). V databáze: DOI: DOI: 10.1103/PhysRevE.95.033308 ; SCOPUS ; WOS ; MLJ: CCC:000396283700007. Kategória publikácie do 2021: ADC Ohlasy: 1. [1] BENALI, Anouar - SHIN, Hyeondeok - HEINONEN, Olle. Quantum Monte Carlo benchmarking of large noncovalent complexes in the L7 benchmark set. In <i>Journal of Chemical Physics</i> , 2020, 153, 19, pp. ISSN 00219606., Registrované v: SCOPUS, WOS, CC Ohlas: zahraničný
V3_06	DUBECKÝ, Matúš. Noncovalent interactions by fixed-node diffusion Monte Carlo: convergence of nodes and energy differences vs gaussian basis-set size. In <i>Journal of chemical theory and computation</i> . Vol. 13, iss. 8 (2017), s. 3626-3635. ISSN 1549-9618 (2017: 5.399 - IF, Q1 - JCR Best Q, 2.497 - SJR, Q1 - SJR Best Q). V databáze: SCOPUS: DOI: 10.1021/acs.jctc.7b00537 ; WOS: CCC:000407522100016 ; MLJ ; CC. Kategória publikácie do 2021: ADC

Ohlasy:

- [1] BENALI, Anouar - LUO, Ye - SHIN, Hyeondeok - PAHLS, Dale - HEINONEN, Olle. Quantum Monte Carlo Calculations of Catalytic Energy Barriers in a Metallorganic Framework with Transition-Metal-Functionalized Nodes. In JOURNAL OF PHYSICAL CHEMISTRY C, 2018, vol. 122, no. 29, pp. 16683-16691. ISSN 1932-7447., Registrované v: SCOPUS, CC, WOS
Ohlas: zahraničný
- [1] ZAHARIEV, F. - GORDON, M. S. Development of a combined quantum monte carlo-effective fragment molecular orbital method. In Molecular Physics, 2019, 117, 9-12, pp. 1532-1540. ISSN 00268976., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
- [1] YANG, D. ChangMo - KIM, Dong Yeon - KIM, Kwang S. Quantum Monte Carlo Study of the Water Dimer Binding Energy and Halogen-pi Interactions. In JOURNAL OF PHYSICAL CHEMISTRY A, 2019, vol. 123, no. 36, pp. 7785-7791. ISSN 1089-5639., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
- [1] KENT, P. R. C. - ANNABERDIYEV, Abdulgani - BENALI, Anouar - BENNETT, M. Chandler - BORDA, Edgar Josue Landinez - DOAK, Peter - HAO, Hongxia - JORDAN, Kenneth D. - KROGEL, Jaron T. - KYLANPAA, Ilkka - LEE, Joonho - LUO, Ye - MALONE, Fionn D. - MELTON, Cody A. - MITAS, Lubos - MORALES, Miguel A. - NEUSCAMMAN, Eric - REBOREDO, Fernando A. - RUBENSTEIN, Brenda - SARITAS, Kayahan - UPADHYAY, Shiv - WANG, Guangming - ZHANG, Shuai - ZHAO, Luning. QMCPACK: Advances in the development, efficiency, and application of auxiliary field and real-space variational and diffusion quantum Monte Carlo. In JOURNAL OF CHEMICAL PHYSICS, 2020, vol. 152, no. 17, pp. ISSN 0021-9606., Registrované v: WOS, CC
Ohlas: zahraničný
- [1] BENALI, Anouar - SHIN, Hyeondeok - HEINONEN, Olle. Quantum Monte Carlo benchmarking of large noncovalent complexes in the L7 benchmark set. In Journal of Chemical Physics, 2020, 153, 19, pp. ISSN 00219606., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
- [1] ERIKSEN, Janus J. The Shape of Full Configuration Interaction to Come. In Journal of Physical Chemistry Letters, 2021, 12, 1, pp. 418-432., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
- [1] ZAHARIEV, F. - GORDON, M. S. Combined quantum Monte Carlo effective fragment molecular orbital method: fragmentation across covalent bonds. In PHYSICAL CHEMISTRY CHEMICAL PHYSICS, 2021, vol. 23, no. 26, pp. 14308-14314. ISSN 1463-9076., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný

V3_07

DUBECKÝ, Matúš - JUREČKA, Petr - MITAS, Luboš - DITTE, Matej - FANTA, Roman. Toward accurate hydrogen bonds by scalable quantum Monte Carlo. In *Journal of chemical theory and computation*. Vol. 15, iss. 6 (2019), s. 3552-3557. ISSN 1549-9618 (2019: 5.011 - IF, Q1 - JCR Best Q, 1.759 - SJR, Q1 - SJR Best Q). V databáze: DOI: 10.1021/acs.jctc.9b00096 ; SCOPUS: 2-s2.0-85066883822 ; WOS: 000471728500011 ; CC: 000471728500011.

Kategória publikácie do 2021: ADC

Ohlasy:

- [1] ZHOU, Xiaojun - ZHAO, Hewang - WANG, Ting - WANG, Fan. Diffusion quantum Monte Carlo calculations with a recent generation of effective core potentials for ionization potentials and electron affinities. In PHYSICAL REVIEW A, 2019, vol. 100, no. 6, pp. ISSN 2469-9926., Registrované v: WOS, CC, SCOPUS
Ohlas: zahraničný
- [1] KLIMEŠ, Jiří - TEW, David P. Efficient and accurate description of adsorption in zeolites. In Journal of Chemical Physics, 2019, 151, 23, pp. ISSN 00219606., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
- [1] NEJAD, Arman - SUHM, Martin A. Concerted Pair Motion Due to Double Hydrogen Bonding: The Formic Acid Dimer Case. In JOURNAL OF THE INDIAN INSTITUTE OF SCIENCE, 2020, vol. 100, no. 1, pp. 5-19. ISSN 0970-4140., Registrované v: WOS, SCOPUS
Ohlas: zahraničný
- [1] MODRZEJEWSKI, Marcin - YOURDKHANI, Sirous - SMIGA, Szymon - KLIMES, Jirí. Random-Phase Approximation in Many-Body Noncovalent Systems: Methane in a Dodecahedral Water Cage. In Journal of Chemical Theory and Computation, 2021, 17, 2, pp. 804-817. ISSN 15499618., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný

V3_08

DUBECKÝ, Matúš - KARLICKÝ, František - MINÁRIK, Stanislav - MITAS, Luboš. Fundamental gap of fluorographene by many-body GW and fixed-node diffusion Monte Carlo methods. In *Journal of Chemical Physics*. Vol. 153, iss. 18 (2020), s. 1-10. ISSN 0021-9606 (2020: 3.488 - IF, Q1 - JCR Best Q, 1.071 - SJR, Q1 - SJR Best Q). V databáze: DOI: 10.1063/5.0030952 ; SCOPUS: 2-s2.0-85096114669 ; WOS: 000593964100001 ; CC: 000593964100001.

Kategória publikácie do 2021: ADC

Ohlasy:

- [1] MORALES-SILVA, Miguel A. - JORDAN, Kenneth D. - SHULENBURGER, Luke - WAGNER, Lucas K. Frontiers of stochastic electronic structure calculations. In Journal of Chemical Physics, 2021, 154, 17, pp. ISSN 00219606., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
- [1] HRUBÝ, Vítězslav - ZDRAŽIL, Lukáš - DŽÍBELOVÁ, Jana - ŠEDAJOVÁ, Veronika - BAKANDRITSOS, Aristeidis - LAZAR, Petr - OTYEPKA, Michal. Unveiling the true band gap of fluorographene and its origins by teaming theory and experiment. In Applied Surface Science, 2022-06-15, 587, pp. ISSN 01694332., Registrované v: SCOPUS, WOS, CC
Ohlas: zahraničný
- [1] OKOTRUB, A. V. - CHEKHOVA, G. N. - PINAKOV, D. V. - YUSHINA, I. V. - BULUSHEVA, L. G. Optical

absorption and photoluminescence of partially fluorinated graphite crystallites. In *Carbon*, 2022-06-30, 193, pp. 98-106. ISSN 00086223., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

4. [1] BARHOUMI, Mohamed - SFINA, Nouredine. Electronic, Optical, and Elastic Properties of CaF₂ Monolayer and Acoustic Phonon Dispersion at Hypersonic Frequencies Using Density Functional Theory and beyond with Random Phase Approximation and Bethe-Salpeter Equation. In *ACS OMEGA*, 2022, vol. 7, no. 18, pp. 15338-15349. ISSN 2470-1343., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

5. [1] BORSE, Rahul Anil - KALE, Manoj B. - SONAWANE, Shirish H. - WANG, Yaobing. Fluorographene and Its Composites: Fundamentals, Electrophysical Properties, DFT Studies, and Advanced Applications. In: *Advanced Functional Materials*, 2022-06-01, 32, 26, pp. ISSN 1616301X., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

6. [1] MALAKOUTIKHAH, Tahereh - HASHEMIFAR, S. Javad - ALAEI, Mojtaba. Novel first-principles insights into graphene fluorination. In: *Journal of Chemical Physics*, 2022-08-07, 157, 5, pp. ISSN 00219606., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

V3_09 FANTA, Roman - KOLESÁR, Vladimír - ŠIMUNEK, Ján - DUBECKÝ, Matúš. Benchmarking lattice energy of a model 1D molecular HF crystal. In *Theoretical Chemistry Accounts*. Vol. 139, iss. 5, (2020), s. 1-4. ISSN 1432-881X (2020: 1.702 - IF, Q4 - JCR Best Q, 0.431 - SJR, Q3 - SJR Best Q). V databáze: DOI: 10.1007/s00214-020-02601-3 ; SCOPUS: 2-s2.0-85083980583 ; WOS: 000529680000001 ; CC: 000529680000001.
Kategória publikácie do 2021: ADC

V3_10 FANTA, Roman - DUBECKÝ, Matúš. Noncovalent Interactions by the Quantum Monte Carlo Method: Strong Influence of Isotropic Jastrow Cutoff Radii. In *Journal of chemical theory and computation*. Vol. 17, iss. 7 (2021), s. 4242-4249. ISSN 1549-9618 (2021: 6.578 - IF, Q1 - JCR Best Q, 1.619 - SJR, Q1 - SJR Best Q). V databáze: DOI: 10.1021/acs.jctc.1c00467 ; SCOPUS: 2-s2.0-85110355430 ; WOS: 000674289800033 ; CC: 000674289800033.
Typ výstupu: článok; Výstup: zahraničný; Kategória publikácie do 2021: ADC

Ohlasy:

1. [1] HOGGAN, Philip E. Quantum Monte Carlo with ground-state input to investigate platinum-doped aluminum catalyst: H-2 production from adsorbed CO. In *NEW ELECTRON CORRELATION METHODS AND THEIR APPLICATIONS, AND USE OF ATOMIC ORBITALS WITH EXPONENTIAL ASYMPTOTES*, 2021, vol. 83, no., pp. 155-170. ISSN 0065-3276., Registrované v: WOS, SCOPUS

Ohlas: zahraničný

V3_11 ŠULKA, Martin - DUBECKÝ, Matúš. Fragmentation of natural orbital occupation numbers-based diagnostic of differential multireference character in complexes with hydrogen bonds. In *Journal of Computational Chemistry*. Vol. 42, iss. 7 (2021), s. 475-483. ISSN 0192-8651 (2021: 3.672 - IF, Q2 - JCR Best Q, 0.778 - SJR, Q1 - SJR Best Q). V databáze: DOI: 10.1002/jcc.26470 ; SCOPUS: 2-s2.0-85097564119 ; WOS: 000598674400001 ; CC: 000612509100002.
Typ výstupu: článok; Výstup: zahraničný; Kategória publikácie do 2021: ADC

I2 Iný výstup publikačnej činnosti ako časť publikácie alebo zborníka

I2_01 ŠULKA, Martin - ŠULKOVÁ, Katarína - DUBECKÝ, Matúš. Assessing the accuracy of quantum Monte Carlo in hydrogen-bonded and strongly correlated systems. In *CESTC 2022 : 18th Central European Symposium on Theoretical Chemistry 2022, 7-10 September 2022, Balatonszárszó, Hungary*. 1. vyd. Budapešť : Hungarian Chemical Society, 2022, S. 90. ISBN 978-615-6018-10-6.
Typ výstupu: časť, ktoré nemožno zaradiť do kategórie V, O, P, U alebo D; Výstup: zahraničný; Kategória publikácie do 2021: AFK

XXX XXX

_01 DUBECKÝ, František - KOVÁČ, Jaroslav - MUDROŇ, Ján - HUBÍK, Pavel - DUBECKÝ, Matúš - GOMBIA, Enos. Photocurrent Spectroscopy of Semi-Insulating GaAs with a New Contact Metallization: Indication of 2DEG Formed at the M-S Interface. In *APCOM 2010. Applied Physics of Condensed Matter : Proceedings of the 16th International Conference. Malá Lučivná, Slovak Republic, 16.-18.6.2010*. Bratislava : Nakladateľstvo STU, 2010, s.29-32. ISBN 978-80-227-3307-6.
Kategória publikácie do 2021: AFD

_02 DUBECKÝ, František - DUBECKÝ, Matúš - MIČUŠÍK, M. - HUBÍK, Pavel - KINDL, D. - GOMBIA, Enos - ŠAGÁTOVÁ, Andrea - NEČAS, Vladimír. M/SI-GaAs/M Devices: Contact Chemistry and Electronic Transport. In *8th Solid State Surfaces and Interfaces : Extended Abstract Book. Smolenice Castle, Slovak Republic, November 25-28, 2013*. Bratislava : Comenius University, 2013, s.42. ISBN 978-80-223-3501-0.
Kategória publikácie do 2021: AFH

_03 DUBECKÝ, František - HUBÍK, Pavel - KINDL, Dobroslav - GOMBIA, Enos - VANKO, Gabriel - ZAŤKO, Bohumír - KOLESÁR, Vladimír - DUBECKÝ, Matúš - BOHÁČEK, Pavol - SEKÁČOVÁ, Mária - ŠAGÁTOVÁ, Andrea - NEČAS, Vladimír. Electronic performance study of Mg-based electrode on semi-insulating GaAs. In *SURFINT - SREN V : 5th Conference on Progress in applied surface, interface and thin film science. Extended abstract book. Florence, Italy. November 20-23, 2017*. Bratislava : Comenius University, 2017, S. 34-35. ISBN 978-80-223-4411-1.
Kategória publikácie do 2021: AFG

DUBECKÝ, Matúš - JUREČKA, Petr - DERIAN, René - HOBZA, Pavel - OTYEPKA, Michal - MITAS, L. Quantum Monte Carlo methods describe noncovalent interactions with subchemical accuracy. In *Journal of chemical theory and computation*. Vol. 9, Iss. 10 (2013), s. 4287-4292. ISSN 1549-9618 (2013: 5.310 - IF, Q1 - JCR Best Q, 2.437 - SJR, Q1 - SJR Best Q).

Ohlasy:

1. [1] LUO, Ye - BENALI, Anouar - SHULENBURGER, Luke - KROGEL, Jaron T. - HEINONEN, Olle - KENT, Paul R. C. Phase stability of TiO₂ polymorphs from diffusion Quantum Monte Carlo. In *NEW JOURNAL OF PHYSICS*, 2016, vol. 18, no., pp. ISSN 1367-2630., Registrované v: SCOPUS, CC, WOS

Ohlas: zahraničný

2. [1] HOJA, Johannes - REILLY, Anthony M. - TKATCHENKO, Alexandre. First-principles modeling of molecular crystals: structures and stabilities, temperature and pressure. In *Wiley Interdisciplinary Reviews: Computational Molecular Science*, 2017, 7, 1, pp. ISSN 1759-0876., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

3. [1] HERMANN, Jan - ALFÈ, Dario - TKATCHENKO, Alexandre. Nanoscale π - π Stacked molecules are bound by collective charge fluctuations. In *Nature Communications*, 2017, 8, ISSN: 2041-1723., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

4. [1] ZHOU, Xiaojun - WANG, Fan. Barrier heights of hydrogen-transfer reactions with diffusion quantum monte carlo method. In *Journal of Computational Chemistry*, 2017, 38, 11, pp. 798-806. ISSN 0192-8651.,

Registrované v: SCOPUS

Ohlas: zahraničný

5. [1] KRONGCHON, Kittithat - BUSEMEYER, Brian - WAGNER, Lucas K. Accurate barrier heights using diffusion Monte Carlo. In *JOURNAL OF CHEMICAL PHYSICS*, 2017, vol. 146, no. 12, pp. ISSN 0021-9606., Registrované v: SCOPUS, CC, WOS

Ohlas: zahraničný

6. [1] HONGO, Kenta - MAEZONO, Ryo. Practical Diffusion Monte Carlo Simulations for Large Noncovalent Systems. In *RECENT PROGRESS IN QUANTUM MONTE CARLO*, 2016, vol. 1234, no., pp. 127-143. ISSN 0097-6156., Registrované v: SCOPUS, WOS

Ohlas: zahraničný

7. [1] HONGO, Kenta - MAEZONO, Ryo. A Computational Scheme To Evaluate Hamaker Constants of Molecules with Practical Size and Anisotropy. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*, 2017, vol. 13, no. 11, pp. 5217-5230. ISSN 1549-9618., Registrované v: SCOPUS, CC, WOS

Ohlas: zahraničný

8. [1] REIMERS, Jeffrey R. - SAJID, A. - KOBAYASHI, Rika - FORD, Michael J. Understanding and Calibrating Density-Functional-Theory Calculations Describing the Energy and Spectroscopy of Defect Sites in Hexagonal Boron Nitride. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*, 2018, vol. 14, no. 3, pp. 1602-1613. ISSN 1549-9618., Registrované v: SCOPUS, CC, WOS

Ohlas: zahraničný

9. [1] KARTASHYNSKA, E. S. - VYSOTSKY, Yu. B. - FAINERMAN, V. B. - VOLLHARDT, D. - MILLER, R. Quantum-chemical analysis of condensed monolayer phases of N-alkanoyl-substituted alanine at the air/water interface. In *COLLOIDS AND SURFACES A-PHYSICO-CHEMICAL AND ENGINEERING ASPECTS*, 2018, vol. 546, no., pp. 346-359. ISSN 0927-7757., Registrované v: SCOPUS, CC, WOS

Ohlas: zahraničný

10. [1] SONG, Suhwan - KIM, Min-Cheol - SIM, Eunji - BENALI, Anouar - HEINONEN, Olle - BURKE, Kieron. Benchmarks and Reliable DFT Results for Spin Gaps of Small Ligand Fe(II) Complexes. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*, 2018, vol. 14, no. 5, pp. 2304-2311. ISSN 1549-9618., Registrované v: SCOPUS, CC, WOS

Ohlas: zahraničný

11. [1] ALLENDORF, Mark D. - HULVEY, Zeric - GENNETT, Thomas - AHMED, Alauddin - AUTREY, Tom - CAMP, Jeffrey - CHO, Eun Seon - FURUKAWA, Hiroyasu - HARANCZYK, Maciej - HEAD-GORDON, Martin - JEONG, Sohee - KARKAMKAR, Abhi - LIU, Di-Jia - LONG, Jeffrey R. - MEIHAUS, Katie R. - NAYYAR, Iffat H. - NAZAROV, Roman - SIEGEL, Donald J. - STAVILA, Vitalie - URBAN, Jeffrey J. - VECCHAM, Srimumkh Prasad - WOOD, Brandon C. An assessment of strategies for the development of solid-state adsorbents for vehicular hydrogen storage. In *ENERGY & ENVIRONMENTAL SCIENCE*, 2018, vol. 11, no. 10, pp. 2784-2812. ISSN 1754-5692., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

12. [1] AL-HAMDANI, Yasmine S. - TKATCHENKO, Alexandre. Understanding non-covalent interactions in larger molecular complexes from first principles. In *Journal of Chemical Physics*, 2019, 150, 1, pp. ISSN 00219606., Registrované v: SCOPUS, WOS, CC

Ohlas: zahraničný

13. [1] WINEMAN-FISHER, Vered - AL-HAMDANI, Yasmine - ADDOU, Iqbal - TKATCHENKO, Alexandre - VARMA, Sameer. Ion-Hydroxyl Interactions: From High-Level Quantum Benchmarks to Transferable Polarizable Force Fields. In *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*, 2019, vol. 15, no. 4, pp. 2444-2453. ISSN 1549-9618.,

Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

14. [1] YANG, D. ChangMo - KIM, Dong Yeon - KIM, Kwang S. Quantum Monte Carlo Study of the Water Dimer Binding Energy and Halogen- π Interactions. In *JOURNAL OF PHYSICAL CHEMISTRY A*, 2019, vol. 123, no. 36, pp. 7785-7791. ISSN 1089-5639., Registrované v: WOS, CC, SCOPUS

Ohlas: zahraničný

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