Tomas Bucko

List of Publications by Year
in descending order

81 papers	4,390 citations	94415 37 h-index	106340 65 g-index
85 all docs	85 docs citations	85 times ranked	5003 citing authors

#	Article	IF	Citations
1	Multiscale Modeling as a Tool for the Prediction of Catalytic Performances: The Case of n-Heptane Hydroconversion in a Large-Pore Zeolite. ACS Catalysis, 2022, 12, 1068-1081.	11.2	21
2	Assessing the Accuracy of Machine Learning Thermodynamic Perturbation Theory: Density Functional Theory and Beyond. Journal of Chemical Theory and Computation, 2022, 18, 1382-1394.	5.3	9
3	Access to sodalite cages in ion-exchanged nanosized FAU zeolites probed by hyperpolarized 129Xe NMR and DFT calculations. Microporous and Mesoporous Materials, 2022, 338, 111965.	4.4	5
4	Methanol carbonylation over acid mordenite: Insights from ab initio molecular dynamics and machine learning thermodynamic perturbation theory. Journal of Catalysis, 2021, 396, 166-178.	6.2	11
5	Hybrid localized graph kernel for machine learning energyâ€related properties of molecules and solids. Journal of Computational Chemistry, 2021, 42, 1390-1401.	3.3	2
6	Understanding the Fundamentals of Microporosity Upgrading in Zeolites: Increasing Diffusion and Catalytic Performances. Advanced Science, 2021, 8, e2100001.	11.2	23
7	Ab initio molecular dynamics investigation of Cs adsorption on Mo(0Â0Â1): Beyond a single monolayer coverage. Applied Surface Science, 2021, 559, 149822.	6.1	4
8	Anharmonic Correction to Adsorption Free Energy from DFT-Based MD Using Thermodynamic Integration. Journal of Chemical Theory and Computation, 2021, 17, 1155-1169.	5.3	29
9	First-principles-informed energy span and microkinetic analysis of ethanol catalytic conversion to 1,3-butadiene on MgO. Catalysis Science and Technology, 2021, 11, 6682-6694.	4.1	4
10	Dynamic Features of Transition States for Î²â€Scission Reactions of Alkenes over Acid Zeolites Revealed by AIMD Simulations. Angewandte Chemie, 2020, 132, 19100-19104.	2.0	9
11	Ab Initio Calculations of Free Energy of Activation at Multiple Electronic Structure Levels Made Affordable: An Effective Combination of Perturbation Theory and Machine Learning. Journal of Chemical Theory and Computation, 2020, 16, 6049-6060.	5.3	28
12	Relative Humidity Facilitated Urea Particle Reaction with Salicylic Acid: A Combined In Situ Spectroscopy and DFT Study. ACS Earth and Space Chemistry, 2020, 4, 1018-1028.	2.7	12
13	Dynamic Features of Transition States for Î²â€Scission Reactions of Alkenes over Acid Zeolites Revealed by AIMD Simulations. Angewandte Chemie - International Edition, 2020, 59, 18938-18942.	13.8	20
14	Computing RPA Adsorption Enthalpies by Machine Learning Thermodynamic Perturbation Theory. Journal of Chemical Theory and Computation, 2019, 15, 6333-6342.	5.3	41
15	Competition of Secondary versus Tertiary Carbenium Routes for the Type B Isomerization of Alkenes over Acid Zeolites Quantified by Ab Initio Molecular Dynamics Simulations. ACS Catalysis, 2019, 9, 9813-9828.	11.2	35
16	On the origin of the difference between type A and type B skeletal isomerization of alkenes catalyzed by zeolites: The crucial input of ab initio molecular dynamics. Journal of Catalysis, 2019, 373, 361-373.	6.2	38
17	Bridging molecular dynamics and correlated wave-function methods for accurate finite-temperature properties. Physical Review Materials, 2019, 3, .	2.4	16
18	Ab initio calculation of the migration free energy of oxygen diffusion in pure and samarium-doped ceria. Physical Review B, 2018, 97, .	3.2	26

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19	On the work function of the surface Mo(0â€‰0â€‰1) and its temperature dependence: an ab initio molecular dynamics study. Journal of Physics Condensed Matter, 2018, 30, 505001.	1.8	3
20	Carbon dioxide capture in 2,2â€²-iminodiethanol aqueous solution fromab initiomolecular dynamics simulations. Journal of Chemical Physics, 2018, 149, 224103.	3.0	7
21	Transition state optimization of periodic systems using delocalized internal coordinates. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	12
22	Effect of alkaline metal cations on the ionic structure of cryolite melts: Ab-initio NpT MD study. Journal of Chemical Physics, 2018, 148, 064501.	3.0	8
23	The dependence on ammonia pretreatment of Nâ‹¯O activation by Co(II) sites in zeolites: a DFT and ab initio molecular dynamics study. Journal of Molecular Modeling, 2017, 23, 160.	1.8	6
24	Carbon dioxide capture in 2-aminoethanol aqueous solution from ab initio molecular dynamics simulations. Journal of Chemical Physics, 2017, 146, .	3.0	9
25	Catalytic conversion of ethanol to 1,3-butadiene on MgO: A comprehensive mechanism elucidation using DFT calculations. Journal of Catalysis, 2017, 346, 78-91.	6.2	70
26	Dissociative iodomethane adsorption on Ag-MOR and the formation of AgI clusters: an ab initio molecular dynamics study. Physical Chemistry Chemical Physics, 2017, 19, 27530-27543.	2.8	41
27	A DFT investigation of the adsorption of iodine compounds and water in H-, Na-, Ag-, and Cu- mordenite. Journal of Chemical Physics, 2016, 144, 244705.	3.0	61
28	On the structure of crystalline and molten cryolite: Insights from the ab initio molecular dynamics in NpT ensemble. Journal of Chemical Physics, 2016, 144, 064502.	3.0	18
29	A Fractionally Ionic Approach to Polarizability and van der Waals Many-Body Dispersion Calculations. Journal of Chemical Theory and Computation, 2016, 12, 5920-5930.	5.3	90
30	C₆ Coefficients and Dipole Polarizabilities for All Atoms and Many Ions in Rows 1â€“6 of the Periodic Table. Journal of Chemical Theory and Computation, 2016, 12, 3603-3613.	5.3	76
31	Catalytic methyl mercaptan coupling to ethylene in chabazite: DFT study of the first C C bond formation. Applied Catalysis B: Environmental, 2016, 187, 195-203.	20.2	13
32	Many-body dispersion corrections for periodic systems: an efficient reciprocal space implementation. Journal of Physics Condensed Matter, 2016, 28, 045201.	1.8	86
33	Negative thermal expansion of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>ScF</mml:mi><mml:mn>3</mml:mn></mml:msub></m Insights from density-functional molecular dynamics in the isothermal-isobaric ensemble. Physical Review B, 2015, 92, .	3.2	34
34	The role of spatial constraints and entropy in the adsorption and transformation of hydrocarbons catalyzed by zeolites. Journal of Catalysis, 2015, 329, 32-48.	6.2	61
35	Extending the applicability of the Tkatchenko-Scheffler dispersion correction via iterative Hirshfeld partitioning. Journal of Chemical Physics, 2014, 141, 034114.	3.0	174
36	Understanding the Adsorption of CuPc and ZnPc on Noble Metal Surfaces by Combining Quantum-Mechanical Modelling and Photoelectron Spectroscopy. Molecules, 2014, 19, 2969-2992.	3.8	69

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37	Improved Density Dependent Correction for the Description of London Dispersion Forces. Journal of Chemical Theory and Computation, 2013, 9, 4293-4299.	5.3	183
38	Effect of the Al Siting on the Structure of Co(II) and Cu(II) Cationic Sites in Ferrierite. A Periodic DFT Molecular Dynamics and FTIR Study. Journal of Physical Chemistry C, 2013, 117, 3958-3968.	3.1	42
39	Tkatchenko-Scheffler van der Waals correction method with and without self-consistent screening applied to solids. Physical Review B, 2013, 87, .	3.2	293
40	Understanding Structure and Bonding of Multilayered Metalâ€“Organic Nanostructures. Journal of Physical Chemistry C, 2013, 117, 3055-3061.	3.1	36
41	Spin crossover transition of Fe(phen)2(NCS)2: periodic dispersion-corrected density-functional study. Physical Chemistry Chemical Physics, 2012, 14, 5389.	2.8	57
42	Simulation of Aqueous Dissolution of Lithium Manganate Spinel from First Principles. Journal of Physical Chemistry C, 2012, 116, 4050-4059.	3.1	57
43	Assessment of ten DFT methods in predicting structures of sheet silicates: Importance of dispersion corrections. Journal of Chemical Physics, 2012, 137, 114105.	3.0	117
44	Van der Waals interactions between hydrocarbon molecules and zeolites: Periodic calculations at different levels of theory, from density functional theory to the random phase approximation and MÃ¸ller-Plesset perturbation theory. Journal of Chemical Physics, 2012, 137, 114111.	3.0	123
45	Ab Initio Study of Structure and Interconversion of Native Cellulose Phases. Journal of Physical Chemistry A, 2011, 115, 10097-10105.	2.5	41
46	Dehydrogenation of propane over ZnMOR. Static and dynamic reaction energy diagram. Journal of Catalysis, 2011, 277, 104-116.	6.2	43
47	Monomolecular cracking of propane over acidic chabazite: An ab initio molecular dynamics and transition path sampling study. Journal of Catalysis, 2011, 279, 220-228.	6.2	98
48	N2O decomposition over Fe-zeolites: Structure of the active sites and the origin of the distinct reactivity of Fe-ferrierite, Fe-ZSM-5, and Fe-beta. A combined periodic DFT and multispectral study. Journal of Catalysis, 2010, 272, 262-274.	6.2	119
49	A density-functional study of the adsorption of methane-thiol on the (111) surfaces of the Ni-group metals: II. Vibrational spectroscopy. Journal of Physics Condensed Matter, 2010, 22, 265006.	1.8	68
50	Entropy effects in hydrocarbon conversion reactions: free-energy integrations and transition-path sampling. Journal of Physics Condensed Matter, 2010, 22, 384201.	1.8	24
51	A density functional study of the adsorption of methane-thiol on the (111) surfaces of the Ni-group metals: I. Molecular and dissociative adsorption. Journal of Physics Condensed Matter, 2010, 22, 265005.	1.8	19
52	Simultaneously Understanding the Geometric and Electronic Structure of Anthraceneselenolate on Au(111): A Combined Theoretical and Experimental Study. Journal of Physical Chemistry C, 2010, 114, 2677-2684.	3.1	34
53	Improved Description of the Structure of Molecular and Layered Crystals: Ab Initio DFT Calculations with van der Waals Corrections. Journal of Physical Chemistry A, 2010, 114, 11814-11824.	2.5	895
54	Mechanism of alkane dehydrogenation catalyzed by acidic zeolites: Ab initio transition path sampling. Journal of Chemical Physics, 2009, 131, 214508.	3.0	55

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55	Molecular adsorption and metal-support interaction for transition-metal clusters in zeolites: NO adsorption on Pdnâ€ˆ(n=1â€“6) clusters in mordenite. Journal of Chemical Physics, 2009, 130, 104503.	3.0	26
56	On the structure and dynamics of secondary n-alkyl cations. Journal of Chemical Physics, 2009, 131, 104314.	3.0	14
57	Electronic Structure of Selfâ€Assembled Monolayers on Au(111) Surfaces: The Impact of Backbone Polarizability. Advanced Functional Materials, 2009, 19, 3766-3775.	14.9	37
58	Interaction of NO molecules with Pd clusters: Ab initio densityâ€“functional study. Journal of Computational Chemistry, 2009, 30, 1910-1922.	3.3	20
59	Effects of Lattice Expansion on the Reactivity of a One-Dimensional Oxide. Journal of the American Chemical Society, 2009, 131, 3253-3259.	13.7	12
60	Activity and Reactivity of Fe2+ Cations in the Zeolite. Ab Initio Free-Energy MD Calculation of the N2O Dissociation over Iron-Exchanged Ferrierite. Journal of Physical Chemistry C, 2009, 113, 18807-18816.	3.1	9
61	Ab initiocalculations of free-energy reaction barriers. Journal of Physics Condensed Matter, 2008, 20, 064211.	1.8	54
62	N2O decomposition on iron exchanged ferrierite. A combined periodic DFT and static IN-SITU FTIR study. Studies in Surface Science and Catalysis, 2008, , 713-716.	1.5	0
63	Adsorption of NO in Fe2+-Exchanged Ferrierite. A Density Functional Theory Study. Journal of Physical Chemistry C, 2007, 111, 586-595.	3.1	37
64	Multiple Adsorption of NO on Fe2+Cations in the Î±- and Î²-Positions of Ferrierite:â€‰ An Experimental and Density Functional Study. Journal of Physical Chemistry C, 2007, 111, 9393-9402.	3.1	41
65	Carbocation Branching Observed in a Simulation. Journal of Physical Chemistry A, 2007, 111, 5945-5947.	2.5	14
66	A DFT Study of Activation of H2 and Ð¡Ð4 over Zn-MOR. Studies in Surface Science and Catalysis, 2007, 172, 397-400.	1.5	0
67	Proton exchange of small hydrocarbons over acidic chabazite: Ab initio study of entropic effects. Journal of Catalysis, 2007, 250, 171-183.	6.2	51
68	Acid-based Catalysis in Zeolites Investigated by Density-Functional Methods. Topics in Catalysis, 2006, 37, 41-54.	2.8	46
69	A DFT study of the adsorption of butane in MOR and activation on the Lewis center. Studies in Surface Science and Catalysis, 2005, 158, 939-946.	1.5	0
70	Ab initio vibrational spectroscopy of molecular adsorbates in mordenite. Studies in Surface Science and Catalysis, 2005, 158, 601-608.	1.5	3
71	Adsorption and Vibrational Spectroscopy of CO on Mordenite:Â Ab initio Density-Functional Study. Journal of Physical Chemistry B, 2005, 109, 7345-7357.	2.6	32
72	Geometry optimization of periodic systems using internal coordinates. Journal of Chemical Physics, 2005, 122, 124508.	3.0	128

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73	Theoretical Investigation of CO Interaction with Copper Sites in Zeolites:Â Periodic DFT and Hybrid Quantum Mechanical/Interatomic Potential Function Study. Journal of Physical Chemistry B, 2005, 109, 9631-9638.	2.6	77
74	A Density Functional Theory Study of Molecular and Dissociative Adsorption of H2on Active Sites in Mordenite. Journal of Physical Chemistry B, 2005, 109, 22491-22501.	2.6	45
75	Periodic DFT Calculations of the Stability of Al/Si Substitutions and Extraframework Zn2+Cations in Mordenite and Reaction Pathway for the Dissociation of H2and CH4. Journal of Physical Chemistry B, 2005, 109, 20361-20369.	2.6	56
76	Adsorption and vibrational spectroscopy of ammonia at mordenite: Ab initio study. Journal of Chemical Physics, 2004, 120, 10263-10277.	3.0	39
77	Ab Initio Simulation of Lewis Sites in Mordenite and Comparative Study of the Strength of Active Sites via CO Adsorption. Journal of Physical Chemistry B, 2004, 108, 13656-13666.	2.6	57
78	Active Sites for the Vapor Phase Beckmann Rearrangement over Mordenite:Â An ab Initio Study. Journal of Physical Chemistry A, 2004, 108, 11388-11397.	2.5	46
79	Defect sites at the (001) surface of mordenite:â€‚ab initiostudy. Journal of Chemical Physics, 2003, 118, 8437-8445.	3.0	22
80	Ab initio density functional investigation of the (001) surface of mordenite. Journal of Chemical Physics, 2002, 117, 7295-7305.	3.0	48
81	Tkatchenko-Scheffler van der Waals correction method with and without self-consistent screening applied to solids. , 0, .		1