

Ab initiomolecular dynamics for open-shell transition m

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Citation Report

#	ARTICLE	IF	CITATIONS
1	Structural and Electronic Properties of Clean and Hydrogenated Diamond (100) Surfaces. Europhysics Letters, 1994, 28, 659-664.	0.7	62
2	Electron-ion dynamics: A technique for simulating both electronic transitions and ionic motion in molecules and materials. Physical Review B, 1994, 50, 18629-18632.	1.1	51
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2006	$\langle i \rangle$ Ab initio study of H-vacancy interactions in fcc metals: Implications for the formation of superabundant vacancies. Physical Review B, 2014, 89, .	1.1	104
2007	Local structures around $\langle i \rangle$ metal dopants in topological insulator $\langle i \rangle$ Bi ₂ Se ₃ states studied	1.1	18
2008	hybridization in the stability of the crystal structure of $\langle i \rangle$ M ₂ O ₃		

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2040	Electronic and spin structure of the topological insulator Bi ₂ Te ₃ <small>xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Te<mml:math /><mml:mrow><mml:mn>2.4</mml:mn></mml:mrow></mml:math>Se<mml:math /><mml:mrow><mml:mn>2.4</mml:mn></mml:mrow></mml:math></small>	1.1	35
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2049	Bulk and surface electron dynamics in a topological insulator <small>xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>p</mml:mi></mml:math>-type</small>	1.1	54
2050	Physical Review B, 2014, 89, . <small>xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>SnSb</mml:mtext></mml:msub></mml:math><mml:msub><mml:mtext>Te</mml:mtext></mml:msub></mml:math></small>	1.1	24

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2070	First-principles study of thermodynamic properties and solubility of aluminum-rare-earth intermetallics. <i>Computational Materials Science</i> , 2014, 90, 56-60.	1.4	22
2071	Role of Hydrogen in Graphene Chemical Vapor Deposition Growth on a Copper Surface. <i>Journal of the American Chemical Society</i> , 2014, 136, 3040-3047.	6.6	234
2072	Twin-boundary segregation energies and solute-diffusion activation enthalpies in Mg-based binary systems: A first-principles study. <i>Scripta Materialia</i> , 2014, 80, 17-20.	2.6	85
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2074	First-principles microscopic model of exchange-driven magnetoelectric response with application to CrO_3 Physical Review B, 2014, 89, .	1.1	11
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2097	Topological transport and atomic tunnellingâ€“clustering dynamics for aged Cu-doped Bi_2Te_3 crystals. <i>Nature Communications</i> , 2014, 5, 5022.	5.8	60
2098	Correlated Optical and Magnetic Properties in Photoreduced Graphene Oxide. <i>Journal of Physical Chemistry C</i> , 2014, 118, 28258-28265.	1.5	21
2099	Incorporation effects of Si in TiC_x thin films. <i>Surface and Coatings Technology</i> , 2014, 258, 392-397.	2.2	17
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2101	Magnetic properties of Fe and Co nanoclusters embedded in the first Cu(100) surface layer. <i>JETP Letters</i> , 2014, 99, 646-649.	0.4	8
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2103	The stabilities and electronic structures of single-layer bismuth oxyhalides for photocatalytic water splitting. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 25854-25861.	1.3	105
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2110	Structural deformation and void formation driven by phase transformation in the $\text{Ge}_2\text{Sb}_2\text{Te}_5$ film. <i>Journal of Materials Chemistry C</i> , 2014, 2, 2001.	2.7	5
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4658	Structural, elastic, and electronic properties of MgB_2C_2 under pressure from first-principles calculations. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26442.	1.0	1
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4676	Defect evolution behaviors from single sulfur point vacancies to line vacancies in monolayer molybdenum disulfide. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 19525-19536.	1.3	6
4677	Metallization of Shock-Compressed Liquid Ammonia. <i>Physical Review Letters</i> , 2021, 126, 025003.	2.9	21
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4680	Multiscale exploration of hydrocarbon adsorption and hopping through ZSM-5 channels "from Monte Carlo modelling to experiment. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 2981-2990.	1.3	4
4681	First-principles formulation of spinel-like structured Li _{4(4x)3x} Y _x Cl ₄ as promising solid-state electrolytes to enable superb lithium ion conductivity and matching oxidation potentials to high-voltage cathodes. <i>Journal of Materials Chemistry A</i> , 2021, 9, 14969-14976.	5.2	9
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4685	Metallic 2H-Tantalum Selenide Nanomaterials as Saturable Absorber for Dual-Wavelength Q-Switched Fiber Laser. <i>Sensors</i> , 2021, 21, 239.	2.1	3
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4694	Tunable electron property induced by B-doping in g-C ₃ N ₄ . <i>RSC Advances</i> , 2021, 11, 15695-15700.	1.7	8
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4702	Exfoliation of boron carbide into ultrathin nanosheets. <i>Nanoscale</i> , 2021, 13, 1652-1662.	2.8	16
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4708	First-principles study of antiferromagnetic cobalt spinels. <i>Current Applied Physics</i> , 2021, 22, 65-70.	1.1	6
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4721	Tailoring submicrometer periodic surface structures via ultrashort pulsed direct laser interference patterning. <i>Physical Review B</i> , 2021, 103, .	1.1	35
4722	Stability and bonding nature of clathrate H cages in a near-room-temperature superconductor <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LaH</mml:mi><mml:mn>10</mml:mn></mml:msub></mml:math> <i>Physical Review Materials</i> , 2021, 5, .	0.9	22
4723	The Role of H ⁺ - and Cu ⁺ -Sites for N ₂ O Formation during NH ₃ -SCR over Cu-CHA. <i>Journal of Physical Chemistry C</i> , 2021, 125, 4595-4601.	1.5	28
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4733	Design principles and physical properties of two-dimensional heterostructured borides. <i>Physical Review Materials</i> , 2021, 5, .	0.9	2
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4735	Acidity and Local Confinement Effect in Mordenite Probed by Solid-State NMR Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 2413-2422.	2.1	17
4736	Construction and Theoretical Calculation of an Ultra-High-Performance LiVPO ₄ /C Cathode by B-Doped Pyrolytic Carbon from Poly(vinylidene Fluoride). <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 15190-15204.	4.0	10

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4738	Localized Nb clusters in U-Nb liquid alloys: An <i>ab initio</i> molecular dynamics study. <i>Nuclear Materials and Energy</i> , 2021, 26, 100915.	0.6	2
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