

Efficient pseudopotentials for plane-wave calculations

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Citation Report

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1	Efficient pseudopotentials for plane-wave calculations. II. Operators for fast iterative diagonalization. Physical Review B, 1991, 43, 8861-8869.	1.1	666
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9925	First-principles-based simulation of interlayer water and alkali metal ions in weathered biotite. <i>Journal of Chemical Physics</i> , 2016, 145, 124703.	1.2	8
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9927	Repulsive tip tilting as the dominant mechanism for hydrogen bond-like features in atomic force microscopy imaging. <i>Applied Physics Letters</i> , 2016, 108, 193102.	1.5	17
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9929	Modeling of neutral-atom scattering at the surface of a crystal for the case of grazing incidence. <i>Journal of Surface Investigation</i> , 2016, 10, 123-127.	0.1	3
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9931	Extremely Large Gate Modulation in Vertical Graphene/WSe ₂ Heterojunction Barristor Based on a Novel Transport Mechanism. <i>Advanced Materials</i> , 2016, 28, 5293-5299.	11.1	92
9932	Theoretical Shaping of Femtosecond Laser Pulses for Molecular Photodissociation with Control Techniques Based on Ehrenfest's Dynamics and Time-Dependent Density Functional Theory. <i>ChemPhysChem</i> , 2016, 17, 1601-1607.	1.0	3
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9935	DFT calculation of NMR $\hat{\nu}$ (¹¹³ Cd) in cadmium complexes. <i>Polyhedron</i> , 2016, 117, 48-56.	1.0	9
9936	Structural and Thermodynamic Properties of the Cm ^{III} Ion Solvated by Water and Methanol. <i>Inorganic Chemistry</i> , 2016, 55, 4992-4999.	1.9	13
9937	Density functional theory study of interaction of graphene with hypoxanthine, xanthine, and uric acid. <i>Molecular Physics</i> , 2016, 114, 2157-2163.	0.8	21
9938	Theoretical study of optical activity of 1:1 hydrogen bond complexes of water with S-warfarin. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 168, 180-189.	2.0	4
9939	Spectroscopic Raman characterization of rutherfordine: a combined DFT and experimental study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 16575-16584.	1.3	43
9940	Gas sensor based on MoS ₂ monolayer. <i>Sensors and Actuators B: Chemical</i> , 2016, 236, 378-385.	4.0	280
9941	A novel theoretical study of thermally-induced reaction and vibration dynamics of methanol dissociative adsorption onto a Si(001) surface. <i>RSC Advances</i> , 2016, 6, 1491-1502.	1.7	5

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9943	Effect of TiO ₂ Nanoparticles on Polyaniline Films Electropolymerized at Different pH. <i>Journal of Physical Chemistry C</i> , 2016, 120, 14977-14983.	1.5	7
9944	The influence of Gaussian strain on sublattice selectivity of impurities in graphene. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 235001.	0.7	4
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9949	Transition-metal-decorated germanene as promising catalyst for removing CO contamination in H ₂ . <i>Materials and Design</i> , 2016, 107, 82-89.	3.3	17
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9951	Novel Au- and Ge-based two-dimensional materials formed through topotactic transitions of AlB ₂ -like structures. <i>Nanoscale</i> , 2016, 8, 13558-13561.	2.8	6
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9955	First-principles prediction of MgB ₂ -like NaBC: A more promising high-temperature superconducting material than LiBC. <i>Solid State Communications</i> , 2016, 233, 30-34.	0.9	7
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9961	Yttrium dispersion on capped carbon nanotube: Promising materials for hydrogen storage applications. <i>International Journal of Hydrogen Energy</i> , 2016, 41, 1053-1059.	3.8	16
9962	Line defects in boron nitride nanostructures: A first-principles study. <i>Solid State Communications</i> , 2016, 234-235, 45-50.	0.9	9
9963	Vertex-Atom-Dependent Rectification in Triangular h-BNC/Triangular Graphene Heterojunctions. <i>Journal of Electronic Materials</i> , 2016, 45, 4484-4490.	1.0	3
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9970	Ultrafast charge-transfer in organic photovoltaic interfaces: geometrical and functionalization effects. <i>Nanoscale</i> , 2016, 8, 15902-15910.	2.8	9
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9973	NMR study and computational assays of meclofenamic Na salt and β -cyclodextrin inclusion complex. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2016, 85, 111-120.	0.9	7
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9980	High Pressure Structural Investigation of Benzoic Acid: Raman Spectroscopy and X-ray Diffraction. <i>Journal of Physical Chemistry C</i> , 2016, 120, 14758-14766.	1.5	60
9981	Hydrogenation of Carbon Monoxide into Formaldehyde in Liquid Media. <i>ACS Sustainable Chemistry and Engineering</i> , 2016, 4, 3970-3977.	3.2	45
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10011	Quantum confinement and dielectric profiles of colloidal nanoplatelets of halide inorganic and hybrid organicâ€“inorganic perovskites. <i>Nanoscale</i> , 2016, 8, 6369-6378.	2.8	136
10012	Exploring Interfacial Events in Gold-Nanocluster-Sensitized Solar Cells: Insights into the Effects of the Cluster Size and Electrolyte on Solar Cell Performance. <i>Journal of the American Chemical Society</i> , 2016, 138, 390-401.	6.6	137
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10021	Enhanced thermoelectric properties of graphene oxide patterned by nanoroads. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 10607-10615.	1.3	14
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10026	A comparative study of low energy radiation responses of SiC, TiC and ZrC. <i>Acta Materialia</i> , 2016, 110, 192-199.	3.8	57
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10054	Pressure-induced phase transformations in amorphous arsenic. <i>Journal of Non-Crystalline Solids</i> , 2016, 437, 6-9.	1.5	0
10055	Behaviour at high pressure of Rb ₇ NaGa ₈ Si ₁₂ O ₄₀ ·3H ₂ O (a zeolite with EDI topology): a combined experimental/computational study. <i>Physics and Chemistry of Minerals</i> , 2016, 43, 209-216.	0.3	12
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11442



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