

1. **The electronic structure of oxygen related defects in PbWO_4 and CaMoO_4 crystals**, *Yonas B. Abraham*, N. A. W. Holzwarth
2. **Quasiparticle Bandstructure of YH_3 and LaH_3** , *J. A. Alford*, M. Y. Chou, Eric Chang, Steven G. Louie
3. **Comparison of Quantum Monte Carlo and Density Functional Models of the Correlation Hole in Second Row Atoms**, *Antonio C. Cancio*, C. Y. Fong
4. **Self-diffusion of adatom on Ni(100) surface**, *C. M. Chang*, C. M. Wei, J. Hafner
5. **Kinetic Energy Functionals for Real Space Calculations**, *Nicholas Choly*, Efthimios Kaxiras
6. **A Theoretical and Experimental Study of Oxomanganese (V) porphyrins. Kinetic Stability is Related to Axial Ligand Acidity**, *Filippo De Angelis*, Roberto Car, Ning Jin and John T. Groves
7. **Half-metallicity in doped perovskite manganites**, *Alexander Dobin*, Renata Wentzcovitch
8. **The F -center in LiF**, *R. B. Dunning*, G. Eric Matthews, N. A. W. Holzwarth, A. R. Tackett
9. **Density functional theory for efficient ab initio molecular dynamics simulations in solution**, *Jean-Luc Fattebert* and François Gygi
10. **Half Metallicity in double perovskite ferromagnets**, *Marco Fornari*, David J. Singh
11. **Quantum-confined Stark effect in semiconductor dots**, *Huaxiang Fu*
12. **Molecular oxygen adsorption on graphene and carbon nanotubes** *P. Giannozzi*, R. Car, G. Scoles
13. **The computing of numeric and analytic Wannier Functions**, *A. Gordienko*, A. S. Poplavnoi
14. **Quantum Monte Carlo Study of Itinerant Ferromagnetism for Mixed Valence Systems**, C. D. Batista, *J. E. Gubernatis*, and J. Bonča
15. **Surface and bulk contributions to the surface optical anisotropy of GaAs and Si**, *PH Hahn*, WG Schmidt, F Bechstedt, C Cobet, K Fleischer, N Esser, J Bernholc

16. **Dynamical Approach to Field Emission of Nanostructures and its Application to Carbon Nanotubes**, *Seungwu Han*, Jisoon Ihm
17. **A DFT-Heisenberg description of V_{15}** , Jens Kortus, *C. Stephen Hellberg*, Mark R. Pederson
18. **Ab initio study of Rhenium Impurities and Vacancies in Nickel-Aluminum Superalloys**, *R. G. Hennig*, M. J. Mills and J. W. Wilkins
19. **Exact time-dependent Kohn-Sham calculations**, *Paul Hessler*, *Jan Werschnik*, Neepa T. Maitra, Kieron Burke
20. **A k -space approach to finite electric fields in insulators**, Ivo Souza, *Jorge Íñiguez* and David Vanderbilt
21. **First-principles study of the stability of BN and C**, *A. Janotti*, S.-H. Wei, D. J. Singh
22. **Theoretical and Computer Simulation Studies of Carbon Nanostructures**, L. Liu, *C.S. Jayanthi*, S.Y. Wu
23. **Quantum Phase Transitions and Stability of Atomic and Molecular Systems**, *Sabre Kais*
24. **Structure and energetics of stoichiometric TiO_2 -anatase surfaces**, *M. Lazzeri*, A. Vittadini, A. Selloni
25. **Revised Information Theory and Similarity Principle Applied to Spin-Spin Correlation**, *Shu-Kun Lin*
26. **Superconductivity in MgB_2 : multiple gaps, anharmonicity, and non-linear electron-phonon coupling**, *Amy Y. Liu*, Igor Mazin, Jens Kortus
27. **Cross-slip paths and energetics in Al and Ag: an *ab initio* study**, *Gang Lu*, Nicholas Kioussis, Vasily V. Bulatov, Efthimios Kaxiras
28. **The Infinite Coupling Strength Limit for the Hooke's Atom**, *Rudolph Magyar*, Kieron Burke
29. **Memory in time-dependent density functional theory**, *Neepa T. Maitra* and Kieron Burke
30. **Variational finite-difference representation of the kinetic energy operator**, *P. Maragakis*, José M. Soler, Efthimios Kaxiras
31. **A new look at treating hydrogen bonding with density functional theory: density consistent molecular basis sets**, *Kristan Markey*, Alexander Wittkopp, and Peter R. Schreiner

32. **Computational Results for the High Pressure Phases of Nitrogen**, *William Mattson*, Richard Martin, Daniel Sanchez-Portal
33. **Large scale *ab initio* investigation of Lithium diffusion in carbon nanotubes**, *Vincent Meunier*, Chris Roland, Jerry Bernholc
34. **Ab initio study of ferroelectric domain walls in PbTiO_3** , *B. Meyer*, David Vanderbilt
35. **Socorro: A modular extensible framework for electronic-structure calculations**, *N. A. Modine*, A. F. Wright, R. A. Lippert, A. Tackett, R. Hatcher
36. **Response with cusp-condition constraints and thermodynamic properties of dense liquid hydrogen**, *K. Nagao*, S. A. Bonev, N. W. Ashcroft
37. **An $O(N)$ real-space method for ab initio quantum transport calculations: application to carbon nanotube-metal contacts**, *Marco Buongiorno Nardelli*, Jerry Bernholc, J.-L. Fattebert
38. **On the possibility of superconductivity at higher temperatures in MgB_2 and related compounds**, *J. B. Neaton* and A. Perali
39. **Internally Contracted Multireference Coupled Cluster Theory: Computer Aided Implementation of advanced electronic structure methods**, *Marcel Nooijen*
40. **Lattice dynamics and elastic properties of corundum (Al_2O_3) by Self-Consistent Atomic Deformation (SCAD) method**, *M. M. Ossowski*, L. L. Boyer, M. J. Mehl, H. T. Stokes
41. **Structural, Electronic, and Magnetic Properties of MnO** , *J.E. Pask*, D.J. Singh, I.I. Mazin, C.S. Hellberg, J. Kortus
42. **Novel nanotubular materials**, *Alex Quandt*, Amy Liu, Ihsan Boustani
43. **Adsorption of Thiol Molecules on $\text{Au}(111)$ Surface**, *Y. Yourdshahyan*, *A. M. Rappe*
44. **Compatible treatment of Berry phase polarization and electric-field linear response**, *Na Sai*, Karin M. Rabe, and David Vanderbilt
45. **First-principles simulations of MgSiO_3 perovskite at lower mantle conditions**, *S. Scandolo*, R. Car
46. **Accurate Calculations of the Peierls Stress in Small Periodic Cells**, *D.E. Segall*, Sohrab Ismail-Beigi, T.A. Arias, Alejandro Strachan and William A. Goddard III

47. **Effects of Substitutions on Superconducting MgB_2** , M.J. Mehl, D.A. Papaconstantopoulos and *David J. Singh*
48. **Wannier functions for attached energy bands**, *Ivo Souza*, Nicola Marzari, David Vanderbilt
49. **Plasmons in Semiconductors from Exchange-Only Calculations**, *J. M. Sullivan*, M. Fuchs, B. C. Larson, A. G. Eguiluz
50. **Prediction of the Temperature-Dependent Conformational Averaging of 1H-NMR Resonances in Vinyl Cyclopropane using Ab Initio Methodology and Boltzmann Statistics**, *Chet W. Swalina*, Guillermo Moyna, Edward O'brien
51. **Comparison of the electronic structures of two phases of the organic conducting material(BEDT-TTF)PF₆**, *Ping Tang*, N. A. W. Holzwarth
52. **How well do Car-Parrinello Simulations reproduce the Born-Oppenheimer surface ?**, *Paul Tangney* and Sandro Scandolo
53. **Car-Parrinello investigation of the motor domain of the muscle protein myosin**, Todd J. Minehardt, *Stanley C. Vozzella*, Nicola Marzari, Ed Pate, Peter A. Kollman, Roger Cooke, Roberto Car
54. **Extracting scattering information from the Kohn-Sham susceptibility**, *Adam Wasserman*, Neepa Maitra, Kieron Burke
55. **Scaling Spin Densities Independently in Density Functional Theory**, *Takeyce K. Whittingham*, Rudolph J. Magyar, Kieron Burke
56. **Geometry optimization for electronically excited states in Similarity Transformed Equation of Motion Coupled Cluster Theory: Application to core-hole localization in core-ionized and core-excited states**, *Mark Wladyslawski* and Marcel Nooijen
57. **DFT study of chemisorption and oxidation of sulfur oxides on Pt(111)**, *Xi Lin*, Kenneth C. Hass, William F. Schneider, Bernhardt L. Trout
58. **Difficulties and challenges in construction of an excited state energy functional**, *Federico Zahariev*, Mel Levy, Kieron Burke
59. **O(N²) First Principle Electronic Structure Calculation: Finite Element Methods with Multigrid Acceleration**, *Peihong Zhang*, Vincent H. Crespi
60. **Manifestation of Electron Correlation Effects in Resonant Inelastic X-ray Scattering of NaV_2O_5** , *G. P. Zhang*, T. A. Callcott, G. T. Woods, L. Lin, Brian Sales, D. Mandrus, and J. He, E. L. Shirley

61. **Dielectric Properties of ZrO₂ within a First-principles Approach,**
Xinyuan Zhao, David Vanderbilt