

pSIC-related papers

1. A. Filippetti and N.A. Spaldin:
Self-interaction-corrected pseudopotential scheme for magnetic and strongly-correlated systems,
Phys. Rev. B **67**, 125109 (2003).
2. B. Van Aken, T. Paalstra, A. Filippetti, and N. A. Spaldin;
Nature Mat. **3**, 164 (2004)
3. C. Toher, A. Filippetti, S. Sanvito, and K. Burke:
Self-interaction errors in density-functional calculations of electronic transport,
Phys. Rev. Lett. **95**, 146402 (2005).
4. A. Filippetti and V. Fiorentini:
Magnetic ordering in CuO from first-principles : a cuprate antiferromagnet with fully three-dimensional exchange interactions,
Phys. Rev. Lett. **95**, 086405 (2005).
5. A. Filippetti and V. Fiorentini:
Double-exchange driven ferromagnetic metal-paramagnetic insulator transition in Mn-doped CuO,
Phys. Rev. B **74**, 220401(R) (2006).
6. A. Filippetti and V. Fiorentini:
Self-interaction-free density-functional band theory for magnetic cuprates,
J. Magn. Magnetic Mat. **310**, 1648 (2007).
7. P. Delugas, V. Fiorentini, A. Filippetti, and G. Pourtois:
Cation charge anomalies and high- κ dielectric behavior in DyScO₃,
Phys. Rev. B **75**, 115126 (2007).
8. A. Filippetti and V. Fiorentini:
Magnetic ordering under strain and spin-Peierls dimerization in GeCuO₃,
Phys. Rev. Lett. **98**, 196403 (2007).
9. G. Colizzi, A. Filippetti, and V. Fiorentini:
Magnetism of La_{0.625}Sr_{0.375}MnO₃ under high-pressure from principles,
Phys. Rev. B **76**, 064428 (2007).
10. A. Filippetti and V. Fiorentini:
Metal-insulator transitions and singlet polarons in one-dimensional Ca_{2+x}Y_{2-x}Cu₅O₁₀,
Phys. Rev. B **77**, 235124 (2008).
11. A. Filippetti, G. M. Lopez, M. Mantega, and V. Fiorentini:
Chain metallicity and antiferro-paramagnetism competition in underdoped YBa₂Cu₃O_{6+x}: a first principles description,
Phys. Rev. B **78**, 233103 (2008)
12. G. Colizzi, A. Filippetti, F. Cossu, and V. Fiorentini:
Interplay of strain and magnetism in La_{1-x}Sr_xMnO₃ from first principles,
Phys. Rev. B **78**, 235122 (2008)
13. D. Puggioni, A. Filippetti, and V. Fiorentini:
Fermi-surface pockets in YBa₂Cu₃O_{6.5} : A comparison of ab initio techniques,
Phys. Rev. B **79**, 064519 (2009)

14. A. Filippetti and V. Fiorentini:
A practical first-principles band-theory approach to the study of correlated materials,
Eur. Phys. J. B **71**, 139 (2009)
free on-line at http://www.epj.org/_pdf/HP_EPJB_practical_first-principles.pdf
15. G. Peralta, D. Puggioni, A. Filippetti, and V. Fiorentini:
Jahn-Teller stabilization of magnetic and orbital ordering in rocksalt CuO,
Phys. Rev. B **80**, 140408(R) (2009)
16. A. Filippetti, D. Puggioni, and V. Fiorentini:
Fermi-surface pockets in magnetic underdoped cuprates from first principles,
Europhys. Lett. **88**, 67009 (2009)
17. G. Colizzi, A. Filippetti, and V. Fiorentini:
Multiferroicity and orbital ordering in Pr_{0.5}Ca_{0.5}MnO₃ from first principles,
Phys. Rev. B **82**, 140101(R) (2010)
18. G. M. Lopez, A. Filippetti, M. Mantega, and V. Fiorentini:
First-principles calculation of electronic and structural properties of YBa₂Cu₃O_{6+y},
Phys. Rev. B **82**, 195122 (2010)
19. P. Delugas, A. Filippetti, V. Fiorentini, D. Fontaine, D. Bilc, and P. Ghosez:
Spontaneous electronic confinement in zero field at band-insulator interfaces,
Phys. Rev. Lett. **106**, 166807 (2011)
20. T. Archer, C.D. Pemmaraju, S. Sanvito, C. Franchini, J. He, A. Filippetti, P. Delugas, D. Puggioni,
V. Fiorentini, R. Tiwari and P. Majumdar:
*Exchange interactions and magnetic phases of transition metal oxides: benchmarking advanced ab
initio methods*,
Phys. Rev. B **84**, 115114 (2011)
21. A. Filippetti, C. D. Pemmaraju, S. Sanvito, P. Delugas, D. Puggioni, and V. Fiorentini:
*Variational pseudo-self-interaction-corrected density-functional approach to the ab-initio description
of correlated solids and molecules*,
Phys. Rev B **85**, in print (2011)
22. D. Puggioni, A. Filippetti, and V. Fiorentini:
Magnetic charge-ordered bad-metal ground state in nickelate superlattices,
Phys. Rev. Lett., submitted (2011)