Publication list

Peer-reviewed journal articles in reverse chronological order

Blue color indicates publications arising from the work done during PhD projects I supervised

1. D. Santos-Cottin, M. Casula, L. de' Medici, F. Le Mardelé, J. Wyzula, M. Orlita, Y. Klein, A. Gauzzi, A. Akrap, R. P. S. M Lobo, *Universal optical features of Dirac cone networks: The case of $BaNiS_2$*, submitted to the Physical Review Letters, under review, arXiv:2104.05521;

2. Tommaso Morresi, Lorenzo Paulatto, Rodolphe Vuilleumier, Michele Casula, *Probing anharmonic phonons by quantum correlators: A path integral approach*, submitted to the Journal of Chemical Physics, arXiv:2103.04094;

3. Tommaso Gorni, Pablo Villar Arribi, Michele Casula, and Luca de' Medici, *Accurate modeling of FeSe with screened Fock exchange and Hund's metal correlations*, submitted to the Physical Review Letters, under review, arXiv:2101.01692;

4. N. Nilforoushan, M. Casula, A. Amaricci, M. Caputo, J. Caillaux, L. Khalil, E. Papalazarou, P. Simon, L. Perfetti, I. Vobornik, P. K. Das, J. Fujii, D. Santos-Cottin, Y. Klein, M. Fabrizio, A. Gauzzi, M. Marsi, *Moving Dirac cones with thermodynamic variables*, submitted to the Proceedings of the National Academy of Sciences, under review, arXiv:1905.12210;

5. Kousuke Nakano, Tommaso Morresi, Michele Casula, Ryo Maezono, Sandro Sorella, *Atomic forces by quantum Monte Carlo: application to phonon dispersion calculation*, Phys. Rev. B **103**, L121110 (2021);

6. N. Nilforoushan, M. Casula, M. Caputo, E. Papalazarou, J. Caillaux, Z. Chen, L. Perfetti, A. Amaricci, D. Santos-Cottin, Y. Klein, A. Gauzzi, and M. Marsi, *Photoinduced renormalization and electronic screening of quasi-two-dimensional Dirac states in $BaNiS_2$*, Phys. Rev. Research **2**, 043397 (2020);

7. Kousuke Nakano, Claudio Attaccalite, Matteo Barborini, Luca Capriotti, Michele Casula, Emanuele Coccia, Mario Dagrada, Claudio Genovese, Ye Luo, Guglielmo Mazzola, Andrea Zen, and Sandro Sorella, *TurboRVB: A many-body toolkit for ab initio electronic simulations by quantum Monte Carlo*, J. Chem. Phys. **152**, 204121 (2020);

8. Blair W. Lebert, Tommaso Gorni, Michele Casula *et al.*, *Epsilon iron as a spin-smectic state*, Proceedings of the National Academy of Sciences **116** (41), 20280 (2019);

9. S. Klotz, M. Casula, K. Komatsu, S. Machida, T. Hattori, *High-pressure structure and electronic properties of YbD_2 to 34 GPa*, Physical Review B **100**, 020101 R (2019);

10. G. Ferlat, M. Hellgren, F.X. Coudert, H. Hay, F. Mauri, M. Casula, *van der Waals forces stabilize low-energy polymorphism in B_2O_3: Implications for the crystallization anomaly*, Physical Review Materials **3**, 063603 (2019);

11. D. Santos-Cottin, Y. Klein, Ph. Werner, T. Miyake, L. de' Medici, A. Gauzzi, R. P. S. M. Lobo, and M. Casula, *Linear behavior of the optical conductivity and incoherent charge transport in $BaCoS_2$*, Physical Review Materials **2**, 105001 (2018);

12. M. T. Entwistle, M. Casula, and R. W. Godby, *Comparison of local density functionals based on electron gas and finite systems*, Physical Review B **97**, 235143 (2018);

13. Jeongnim Kim, Andrew D. Baczewski *et al.*, *QMCPACK: an open source ab initio quantum Monte Carlo package for the electronic structure of atoms, molecules and solids*, Journal of Physics: Condensed Matter **30**, 195901 (2018);

14. Nicolas Dupuy, and Michele Casula, *Fate of the open-shell singlet ground state in the experimentally accessible acenes: A quantum Monte Carlo study*, The Journal of Chemical Physics **148**, 134112 (2018);

15. Yannick Klein, Michele Casula, David Santos-Cottin, Alain Audouard, David Vignolles, Gwendal Fève, Vincent Freulon, Bernard Plaçais, Marine Verseils, Hancheng Yang, Lorenzo Paulatto, and Andrea Gauzzi, *Importance of nonlocal electron correlation in the $BaNiS_2$ semimetal from quantum oscillations studies*, Physical Review B **97**, 075140 (2018);

16. Félix Mouhat, Sandro Sorella, Rodolphe Vuilleumier, Marco Saitta, and Michele Casula, *Fully Quantum Description of the Zundel Ion: Combining Variational Quantum Monte Carlo with Path Integral Langevin Dynamics*, Journal of Chemical Theory and Computation **13**, 2400 (2017);

17. Mario Dagrada, Seher Karakuzu, Verónica Laura Vildosola, Michele Casula, and Sandro Sorella, *Exact special twist method for quantum Monte Carlo simulations*, Physical Review B **94**, 245108 (2016);

18. Brian Busemeyer, Mario Dagrada, Sandro Sorella, Michele Casula, and Lucas K. Wagner, *Competing collinear magnetic structures in superconducting FeSe by first- principles quantum Monte Carlo calculations*, Physical Review B **94**, 035198 (2016);

19. Philipp Werner, and Michele Casula, *Dynamical screening in correlated electron systems – from models to realistic materials*, Journal of physics: Condensed Matter **28**, 383001 (2016);

20. David Santos-Cottin, Michele Casula, Gabriel Lantz, Yannick Klein, Luca Petaccia, Patrick Le Févre, François Bertran, Evangelos Papalazarou, Marino Marsi, and Andrea Gauzzi. *Rashba coupling amplification by a staggered crystal field*, Nature Communications **7**, 11258 (2016);

21. David Santos-Cottin, Andrea Gauzzi, Marine Verseils, Benoit Baptiste, Gwendal Feve, Vincent Freulon, Bernard Plaçais, Michele Casula, and Yannick Klein, *Anomalous metallic state in quasi-2D BaNiS2*, Phys. Rev. B **93**, 125120 (2016);

22. F. Decremps, G. Morard, G. Garbarino, and M. Casula, *Polyamorphism of a Ce-based bulk metallic glass by high-pressure and high-temperature density measurements*, Phys. Rev. B **93**, 054209 (2016);

23. S. Sorella, N. Devaux, M. Dagrada, G. Mazzola, and M. Casula, *Geminal embedding scheme for optimal atomic basis set construction in correlated calculations*, J. Chem. Phys. **143**, 244112 (2015);

24. H. Hay, G. Ferlat, M. Casula, A. P. Seitsonen, and F. Mauri, *Dispersion effects in SiO2 polymorphs: An ab initio study*, Phys. Rev. B **92**, 144111 (2015);

25. N. Dupuy, Samira Bouaouli, Francesco Mauri, Sandro Sorella, and Michele Casula, *Vertical and adiabatic excitations in anthracene from quantum Monte Carlo: Constrained energy minimization for structural and electronic excited-state properties in the JAGP ansatz*, J. Chem. Phys. **142**, 214109 (2015);

26. N. Devaux, M. Casula, F. Decremps, S. Sorella, *Electronic origin of the volume collapse in Cerium*, Physical Review B **91**, 081101(R) (2015);

27. Ambroise van Roekeghem, Thomas Ayral, Jan M. Tomczak, Michele Casula, Nan Xu, Hong Ding, Michel Ferrero, Olivier Parcollet, Hong Jiang, Silke Biermann, *Dynamical correlations and screened exchange on the experimental bench: spectral properties of the cobalt pnictide $BaCo_2As_2$*, Physical Review Letters **113**, 266403 (2014);

28. Jan M. Tomczak, M. Casula, T. Miyake, and S. Biermann, *Asymmetry in band widening and quasiparticle lifetimes in SrVO3: Competition between screened exchange and local correlations from combined GW and dynamical mean-field theory GW + DMFT*, Phys. Rev. B **90**, 165138 (2014);

29. Gianluca Giovannetti, Michele Casula, Philipp Werner, Francesco Mauri, and Massimo Capone, *Downfolding electron-phonon Hamiltonians from ab initio calculations: Application to K3 picene*, Phys. Rev. B **90**, 115435 (2014);

30. Mario Dagrada, Michele Casula, Antonino M. Saitta, Sandro Sorella, and Francesco Mauri, *Quantum Monte Carlo Study of the Protonated Water Dimer*, J. Chem. Theory Comp. **10**, 1980 (2014);

31. Michele Casula, Sandro Sorella *Improper s-wave symmetry of the electronic pairing in iron-based superconductors by first-principles calculations*, Phys. Rev. B **88**, 155125 (2013);

32. V. Brouet, Ping-Hui Lin, Y. Texier, J. Bobroff, A. Taleb-Ibrahimi, P. Le Fèvre, F. Bertran, M. Casula, P. Werner, S. Biermann, F. Rullier-Albenque, A. Forget, and D. Colson, *Large Temperature Dependence of the Number of Carriers in Co-Doped $BaFe_2As_2$*, Phys. Rev. Lett. **110**, 167002 (2013);

33. Jan M. Tomczak, Michele Casula, Takashi Miyake, Ferdi Aryasetiawan, Silke Biermann, *Combined GW and dynamical mean field theory: Dynamical screening effects in transition metal oxides*, Europhysics Letters **100**, 67001 (2012);

34. M. Casula, Ph. Werner, L. Vaugier, F. Aryasetiawan, T. Miyake, A. J. Millis, and S. Biermann, *Low-Energy Models for Correlated Materials: Bandwidth Renormalization from Coulombic Screening*, Phys. Rev. Lett. **109**, 126408 (2012);

35. Michele Casula, Matteo Calandra, and Francesco Mauri, *Local and nonlocal electron-phonon couplings in K_3 picene and the effect of metallic screening*, Phys. Rev. B **86**, 075445 (2012);

36. Philipp Werner, Michele Casula, Takashi Miyake, Ferdi Aryasetiawan, Andrew J. Millis, and Silke Biermann, *Satellites and large doping and temperature dependence of electronic properties in hole-doped* $BaFe_2As_2$, Nature Physics **8**, 331 (2012);

37. Michele Casula, Alexey Rubtsov, and Silke Biermann *Dynamical screening effects in correlated materials: Plasmon satellites and spectral weight transfers from a Green's function ansatz to extended dynamical mean field theory*, Physical Review B **85**, 035115 (2012);

38. Michele Casula, Matteo Calandra, Gianni Profeta, and Francesco Mauri, *Intercalant and Intermolecular Phonon Assisted Superconductivity in K-Doped Picene*, Physical Review Letters **107**, 137006 (2011);

39. N. Helbig, J.I. Fuks, M. Casula, M.J. Verstraete, M.A.L. Marques, I.V. Tokatly, A. Rubio, *Density functional theory beyond the linear regime: Validating adiabatic LDA*, Physical Review A **83**, 032503 (2011);

40. Sandro Sorella, Michele Casula, Leonardo Spanu, Andrea Dal Corso, *Ab-initio calculations for the beta-tin diamond transition in Silicon: comparing theories with experiments*, Physical Review B **83**, 075119 (2011);

41. M. Casula, S. Moroni, C. Filippi, S. Sorella, *Size-consistent variational approaches to non-local pseudopotentials: standard and lattice regularized diffusion Monte Carlo methods revisited*, Journal of Chemical Physics **132**, 154113 (2010);

42. B. Clark, M. Casula, D. M. Ceperley, *Hexatic and Mesoscopic Phases in a 2D Quantum Coulomb System*, Physical Review Letters **103**, 055701 (2009);

43. M. Marchi, S. Azadi, M. Casula, S. Sorella, *Resonating Valence Bond wave function with molecular orbitals: application to first-row molecules*, J. Chem. Phys. **131**, 154116 (2009);

44. M. Casula, M. Marchi, S. Azadi, S. Sorella, *A consistent description of the iron dimer spectrum with a correlated single-determinant wave function*, Chemical Physics Letters **477**, Issues 4-6, 255 (2009);

45. L. Shulenburger, M. Casula, G. Senatore, and R. M. Martin, *Spin resolved energy parametrization of a quasi-one-dimensional electron gas*, Journal of Physics A, Mathematical and theoretical **42**, Issue 21, 214021 (2009);

46. M. Casula, D. M. Ceperley, and Erich J. Mueller, *Quantum Monte Carlo study of one dimensional trapped fermions with attractive contact interactions*, Phys. Rev. A **78**, 033607 (2008);

47. L. Shulenburger, M. Casula, G. Senatore, and R. M. Martin, *Correlation effects in quasi one dimensional electron wires*, Phys. Rev. B **78**, 165303 (2008);

48. Todd D. Beaudet, Michele Casula, Jeongnim Kim, Sandro Sorella, and Richard M. Martin, *Molecular hydrogen adsorbed on benzene: insights from a quantum Monte Carlo study*, J. Chem. Phys. **129**, 164711 (2008);

49. S. Sorella, M. Casula, and D. Rocca, *Weak binding between two aromatic rings: feeling the van der Waals attraction by quantum Monte Carlo methods*, J. Chem. Phys. **127**, 014105 (2007);

50. M. Casula, S. Sorella, and G. Senatore, *Ground state properties of the one-dimensional Coulomb gas using the lattice regularized diffusion Monte Carlo*, Phys. Rev. B **74**, 245427 (2006);

51. M. Casula, *Beyond the locality approximation in the standard diffusion Monte Carlo method*, Phys. Rev. B **74**, 161102 R (2006);

52. M. Casula, and G. Senatore, *Charge and spin correlation of a one dimensional electron gas on the continuum*, Chem. Phys. Chem. **6**, 1902 (2005);

53. M. Casula, C. Filippi, S. Sorella, *Diffusion Monte Carlo with Lattice Regularization*, Phys. Rev. Lett. **95**, 100201 (2005);

54. M. Casula, C. Attaccalite and S. Sorella, *Correlated geminal wave function for molecules: an efficient resonating valence bond approach*, J. Chem. Phys. **121**, 7110 (2004);

55. M. Casula and S. Sorella, *Geminal wave function with Jastrow correlation: a first application to atoms*, J. Chem. Phys. **119**, 6500 (2003).

Peer-reviewed conference proceedings

1. M. Casula, S. Yunoki, C. Attaccalite, S. Sorella, *Resonating Valence Bond Wave Function: from lattice models to realistic systems*, for the proceedings of the "Conference on Computational Physics, CCP 2004", Computer Physics Communications **169**, Issues 1-3, 386 (2005).