List of publications of Claudio Verdozzi

Articles published in scientific journals

Articles submitted

49. M. Hopjan, E. Perfetto, G. Stefanucci, and C. Verdozzi, *Molecular Junctions and Molecular Motors: Including Electronic Correlations via Nonequilibrium Green's Functions*, submitted to Physical Review Letters, and arXiv:1712.08061.

48. D. Karlsson, M. Hopjan, and C. Verdozzi, *Systems with disorder, interactions, and out of equilibrium: The exact independent-particle picture from density functional theory*, submitted to Physical Review Letters, and arXiv:1707.04216.

Peer-reviewed articles

47. E. Boström, A. Mikkelsen, C. Verdozzi, E. Perfetto, and G. Stefanucci, *Charge separation in donor-C60 complexes with real-time Green's functions: The importance of nonlocal correlations*, accepted for publication in Nano Letters.

46. E. Mårsell, E. Boström, A. Harth, A. Losquin, C. Guo, Y.-C. Cheng, E. Lorek, S. Lehmann, G. Nylund, M. Stankovski, C. L. Arnold, M. Miranda, K. A. Dick, J. Mauritsson, C. Verdozzi, A. L'Huillier, and A. Mikkelsen, *Spatial Control of Multiphoton Electron Excitations in InAs Nanowires by Varying Crystal Phase and Light Polarization*, accepted for publication in Nano Letters.

45. M. Hopjan, D. Karlsson, S. Ydman, C. Verdozzi, and C.-O. Almbladh, *Merging features from Green's functions and time dependent density functional theory: A route to the description of correlated materials out of equilibrium?*, Phys. Rev. Lett. **116**, 236402 (2016).

44. E. Boström, A. Mikkelsen, and C. Verdozzi, *Time-resolved spectroscopy at surfaces and adsorbate dynamics: insights from a model-system approach*, Phys. Rev. B **93**, 195416 (2016).

43. N. Schlünzen, S. Hermanns, M. Bonitz, C. Verdozzi, *Dynamics of strongly correlated fermions: Ab ini o results for two and three dimensions*, Phys. Rev. **93** , 035107 (2016).

42. D. Karlsson and C. Verdozzi, *Transport of Correlated Electrons through Disordered Chains: A Perspective on Entanglement, Conductance, and Disorder Averaging*, Phys. Rev. B **90**, 201109(R), (2014).

41. M. Hopjan and C. Verdozzi, *Probing Strongly Correlated Materials in Nonequilibrium: Basic Concepts and Possible Future Trends in First Principle Approaches* , Topics in Current Chemistry **347**, 347 (2014).

40. A. Kartsev, C. Verdozzi, G. Stefanucci, *Nonadiabatic Van der Pol oscillations in molecular transport*, The European Physical Journal B **87**, 1 (2014)

39. A. Kartsev, D. Karlsson, A. Privitera, C. Verdozzi, *Three-dimensional dynamics of a fermionic Mott wedding-cake in clean and disordered optical lattices*, Sci. Rep. 3, 2570 (2013).

38. V. Vettchinkina, A. Kartsev, D. Karlsson, C. Verdozzi, *Interacting fermions in 1D disordered lattices: Exploring localization and transport properties with lattice density-functional theories*, Phys. Rev. B, 115115 (2013).

37. D. Karlsson, A. Privitera and C. Verdozzi, *Time Dependent Density Functional Theory meets Dynamical Mean Field Theory: Real-Time Dynamics for the 3D Hubbard Model*, Phys. Rev. Lett. 106, 116401 (2011).

36. M. Puig von Friesen, C. Verdozzi, C.-O. Almbladh, *Can we always get the entanglement entropy from the Kadanoff-Baym equations? The case of the T-matrix approximation*, EPL 95, 27005 (2011).

35. C. Verdozzi, D. Karlsson, M. Puig von Friesen, C.-O. Almbladh, U. von Barth, *Some open questions in TDDFT: Clues from lattice models and Kadanoff-Baym dynamics*, Chemical Physics 391, 37 (2011).

34. D. Karlsson, C. Verdozzi, M. M. Odashima and K. Capelle, *Dynamical melting of the Mott insulator: Time evolution of the density and entropy of out-of-equilibrium cold fermion gases*, EPL 93, 23003 (2011).

33. M. Puig von Friesen, C. Verdozzi, C.-O. Almbladh, *Kadanoff-Baym description of Hubbard clusters out of equilibrium: performance of many-body schemes, correlation-induced damping and multiple quasi-steady states*, Phys. Rev. B 82, 155108 (2010).

32. S. Kurth, G. Stefanucci, E. Koshravi, C. Verdozzi and E. K. U. Gross, *Dynamical Coulomb Blockade and the Derivative Discontinuity of Time-Dependent Density Functional Theory*, Editor's choice, Phys. Rev. Lett. 104, 236801 (2010).

31. M. Puig von Friesen, C. Verdozzi, C.-O. Almbladh, *Successes and failures of Kadanoff-Baym dynamics in Hubbard nanoclusters*, Phys. Rev. Lett. 103, 176404 (2009).

30. C.Verdozzi, *"Time-Dependent-Density-Functional-Theory and Strongly Correlated Systems: Insight From Numerical Studies*, Phys. Rev. Lett. 101, 166401 (2008)

29. P. Samuelsson and C.Verdozzi, *" Two-particle Spin Entanglement in Magnetic Anderson Nanoclusters"*, Phys.Rev. B 75, 132405 (2007).

28. C. Verdozzi, G. Stefanucci, C.-O. Almbladh, *"Classical Nuclear Motion in Quantum Transport"*, Phys. Rev. Lett. 97, 046603 (2006).

27. M. Larsson, E. S. Moskalenko, L. A. Larsson, P. O. Holtz, C.Verdozzi C. O. Almbladh, W. V. Schoenfeld and P. M. Petroff, *" Magnetic field effects on optical and transport properties in InAs/GaAs quantum dots"*, Phys. Rev. B 74, 245312 (2006).

26. Y. Luo. C. Verdozzi, N. Kioussis, *Tunable Doniach phase diagram for strongly-correlated nanoclusters* Phys. Rev. B 71, 033304 (2005).

25. C.Verdozzi, N.Kioussis and Y.Luo *Disordered Kondo nanoclusters: Effect of energy spacing* , Phys.Rev.B 70, 132404 (2004).

24. Y.Luo. C. Verdozzi, N.Kioussis, *Zero-temperature phase diagram for strongly correlated nanochains*, J.Appl.Phys. 95, 7198 (2004).

23. C.Verdozzi, P.A.Schultz, R.Wu, A.H.Edwards and N.Kioussis, *Layer intermixing during metal/metal-oxide adsorption: Ti/Sapphire (0001)*, Phys. Rev. B 66, 125408 (2002).

22. E.M.King, S.J.Clark,C.Verdozzi,G.J.Ackland, *Interaction between metallic p orbitals and the p orbitals of organic molecules: the binding between ethylene and aluminum*, Journal of physical Chemistry B 105, 641 (2001).

21. C.Verdozzi, M.Cini, A.Marini,*Auger Spectroscopy of Strongly Correlated Systems: present status and future trends*, J. of Electron Spectroscopy and Related Phenomena, 117-118, 41(2001).

20. C,Verdozzi, D.R.Jennison, P. A. Schultz, M. P.Sears, *The sapphire (0001) surface, clean and with d-metal overlayers* , Phys.Rev.Letters 82, 799 (1999).

19. D. R. Jennison, C.Verdozzi, P. A. Schultz, M. P.Sears, *Ab initio structural predictions for ultrathin Al_2O_3 films on metallic substrates*, Phys.Rev.B59, R15605 (1999).

18. C. Verdozzi , D. Jennison, P. Schultz, M. P.Sears, J. C. Barbour and B. G. Potter, *Unusual structural relaxation for Rare Earth impurities in Sapphire: an ab initio study of Lanthanum*, Phys.Rev.Letters 80, 5615 (1998).

17. J.Cole, B.Frederick, J.Power, C.Perry, Q. Chen, C.Verdozzi,N.Richardson, P.Weightman, *Orientation of Molecular Adsorbates from Reflection Anisotropy Spectroscopy*, Phys.Stat.sol.(a) 170, 235 (1998).

16. B.Frederick, J.Cole, J.Power, C.Perry, Q. Chen, N.Richardson, P.Weightman, C.Verdozzi, D.Jennison, P.Schultz, M.Sears,*Molecular orientation with visible light: RAS of 3-thiophene carboxylate on Cu(110) surfaces*, Phys. Rev. B 58, 10883 (1998)

15. C.Verdozzi, P.J.Durham, J.R.Cole, P.Weightman, *Correlation and disorder effects in photoelectron and Auger spectra: The late transition metals and their alloys*, Phys. Rev.B 55, 16143 (1997).

14. C.Verdozzi,M.Cini,*Extended Hubbard Model with Off-site Interactions: Two particle spectrum and Auger spectroscopy*, Phys.Rev B 51, 7412 (1995).

13. C.Verdozzi, *The role of off-site interactions in the theory of CVV Auger spectra in solids*, J. of El. Spectroscopy and Related Phenomena 72, 141 (1995).

12. M.Cini,A.D'Andrea and C.Verdozzi, *Many-Photon Effects in inelastic light scattering: theory and model applications*, International Journal of Modern Physics B 9 ,1185 (1995).

11. C.Verdozzi, R.W.Godby, S.Holloway,*Evaluation of GW approximations for the self-energy of a Hubbard Cluster*, Phys. Rev. Lett. 74, 2327 (1995).

10. P.Weightman, R.J.Cole, C.Verdozzi and P.Durham,*Influence of Matrix Elements Effects in the Density of States from Photoemission Spectra CuPd Alloy*, Phys.Rev.Letters 72, 793 (1994).

9. R.J.Cole, C.Verdozzi, M.Cini, P.Weightman, *Offsite interactions in the CVV Auger spectrum of noble metals: A study of Silver,* Phys. Rev. B 49, 13329 (1994).

8. M.Cini, A.D'Andrea and C.Verdozzi, *Many-Photon Effects in inelastic light scattering*, Physic Letters A 180, 430 (1993).

7. M.Cini and C.Verdozzi, *The role of offsite interactions in Auger line shape analysis from closed bands systems*, Physica Scripta T41, 67 (1992).

6. C.Verdozzi, M.Cini, J.F.McGilp, G.Mondio, D.Norman, J.A.Evans, A.D.Laine, P.S.Fowles, L.Duo' and P.Weightman, *The $N_{67}O_{45}O_{45}$ Auger spectrum of metallic Au*, Phys.Rev. B 43, 9550 (1991).

5. C.Verdozzi, M.Cini, J.A.Evans, R.J.Cole, A.D.Laine, P.S.Fowles, L.Duo', and P.Weightman, *Off-site contributions to Electron Correlation; an extension to the Hubbard model studied by Auger spectroscopy*, Europhys. Lett.16, 743 (1991).

4. M.Cini, M. De Crescenzi, F.Patella, N.Motta, M.Sastry, F.Rochet, R.Pasquali, A.Balzarotti, C.Verdozzi, *Palladium clusters on graphite: evidence of resonant hybrid states in the valence and conduction bands*, Phys. Rev. B4, 15685 (1990).

3. M.Cini, C.Verdozzi, *Photoemission and Auger spectra of incompletely filled bands: intermediate coupling theory and application to palladium metal*, J.Phys.Cond.Matter 1, 7457 (1989).

2. M.Cini C.Verdozzi, *Many body effects in the Electron Spectroscopies of Incompletely filled bands*, Il Nuovo Cimento 9D, 1 (1987).

1. M.Cini, C.Verdozzi, *Photoemission and Auger spectra of partially filled bands: a cluster approach*, Solid State Comm. 57 657 (1986).

Conferences and Symposia

9. D. Karlsson and C. Verdozzi, *Effective bias and potentials in steady-state quantum transport: A NEGF reverse-engineering study*, J. Phys. Conf. Ser, **696**, 012018 (2016).

8. D. O. Winge, M. Franckie, C. Verdozzi, A. Wacker and M. F. Pereira *Simple electron-electron scattering in non-equilibrium Greens function simulations* J. Phys. Conf. Ser, **696**, 012013 (2016).

7. E. Boström, M. Hopjan, A. Kartsev, C. Verdozzi, and C.-O. Almbladh, *Nonequilibrium Green's functions and atom-surface dynamics: Simple views from a simple model system*, J. Phys. Conf. Ser, **696**, 012007 (2016)

6. M. Puig von Friesen, C. Verdozzi, C.-O. Almbladh, *Articial damping in the Kadanoff-Baym dynamics of small Hubbard chains*, J. Phys: Conf. Ser. 220, 012016 (2010).

5. N.Kioussis, Y.Luo. C. Verdozzi, in Physics of Spins in Solids: Materials, Methods, and Applications, S.Halilov ed, p.115-138, NSS Mathematics, Physics and Chemistry Vol.156 Kluwer (2004).

4. G.J.Ackland and C.Verdozzi, *Speeding up ab initio molecular dynamics by Semi-empirical Potentials* Abstract Book of the MRS Fall Meeting, symposium D, p.65 (1999).

3. M.Cini,A.D'Andrea,R.Del Sole,L.Reining, C.Verdozzi, R.Girlanda, E.Piparo and D.Weaire, *Nonlinear Optical Response of Surfaces and Interfaces* in *EPIOPTICS*, edited by J. McGilp, Springer Verlag, 1995 (Berlin).

2. C.Verdozzi, *Solid state perspective in the theory of Auger decay*, in (e,2e) and related processes NATO ASI series, Academic Publishers, Holland (1993)

1. M.Cini, C.Verdozzi,*Correlation effects in Photoemission and Auger spectrum of Palladium*, Springer series in Surface science 18, Eds. G.Cubiotti, G.Mondio, K.Wandelt, Springer-Verlag Berlin (1989).

Monographs

1. C.Verdozzi, *Exact diagonalization studies of strongly correlated clusters*, Lecture notes for the Doctorate Programme in Materials Science, University of Milano-Bicocca, Italy (2005).

Other publications

Papers that are available on the Los-Alamos preprint archive http://xxx.lanl.gov/

2. M. Puig von Friesen, C. Verdozzi, C.-O. Almbladh, *Kadanoff-Baym equations and approximate double occupancy in a Hubbard dimer*, arXiv:1009.2917

1. C.Verdozzi and C.-O Almbladh *Lanczos-adapted time evolution for open boundary quantum transport*, arXiv:0808.1643