

## Claudio Verdozzi's research profile

My research activity, started with the theoretical study of electron (Auger, Photoemission) spectroscopy. I i) introduced a supercell approach to deal with disorder and correlations in the late transition metal alloys [1], ii) provided a unitary description of the spectroscopical behavior of supported Pd transition metal clusters [2], iii) extended the theory of the Auger decay in solids to the case of long ranged final state interactions [3, 4] iv) proposed a scheme for a partial cancellation of self-energy and vertex corrections for short range interactions [5]. I then proposed a theoretical scheme to describe many-photon effects in inelastic light scattering phenomena [6], with the electron-photon coupling included to all orders. Model results showed the interesting effect of a dynamical Stark effect contribution to the second harmonic generation response. My interest in correlated systems led me to consider the adequacy of the GW approximation for strongly correlated systems [7] performing for the first time comparisons between exact and GW solutions. Later, I became interested in metal oxides surfaces and performed the first large-scale *ab-initio* Density-Functional studies for aluminum oxide-related systems [8, 9, 10]. I studied isolated La impurities in a sapphire matrix [8], and my theoretical predictions have been confirmed in several experiments. My work on the (0001) surface [9] characterized in detail for the first time the nature of the clean surface and the metal-sapphire interface and also qualified the nature of the ad-metal growth. I have also developed and implemented a temporal embedding scheme to switch on the fly between *ab-initio* and semi-empirical potentials, to reduce the computational effort in molecular dynamics [11]. In the past few years, I developed a general-purpose, exact diagonalization code and used it to study Kondo-type nanoclusters [12, 13], providing the first example of a “Doniach phase diagram” for a nanocluster with regions of prevailing Kondo or RKKY correlations. I used the same approach to perform the first study of entanglement in periodic Anderson clusters, obtaining an entanglement phase diagram and addressing the effect of charge fluctuations [14].

Since in Lund, my activity has been primarily devoted to the study of non equilibrium phenomena. In 2007, I introduced a Time-Dependent Density Functional Theory (TDDFT) description for strongly correlated finite systems in non equilibrium [15], which was then applied to cold fermion atoms in optical lattices [16]. Then, using Dynamical Mean Field Theory, I have introduced a new class of exchange-correlation potentials to describe via TDDFT the 3D Hubbard model out of equilibrium [17] and, very recently, also the generalization to the presence of electron-phonon interactions, i.e. (TD)DFT for the Hubbard-Holstein model [18]. In the area of transport phenomena, I i) proposed an *ab-initio* quantum-classical mixed scheme to study nuclear dynamics in quantum transport [19]. With it, I provided the first example of current-induced molecular desorption as obtained from a full time-dependent approach and suggested the use of ac biases as a way to tailor electromigration. The results also showed the importance of nonadiabatic effects for ultrafast phenomena in nanodevices ii) I presented a time-dependent picture of Coulomb Blockade based on TDDFT, and investigated the relevance of a discontinuity in the exchange-correlation potential in molecular transport [20]. Another line of investigation I have recently pursued is the non equilibrium dynamics of strongly correlated clusters, in terms of many-body approximations within the framework of the Kadanoff-Baym equations [21]. This has provided insight into some basic shortcoming of many-body self-consistent approximations based on infinite partial summations, which remain also for clusters contacted to infinite reservoirs [22]. The NEGF approach has been recently applied to the dynamics of ultracold fermions in optical lattices [30], for opening-trap geometries.

I have also focussed on a description of the competing role of interactions and disorder in transport [23, 24] and in cold atom [28] phenomena, and used Density Functional Theory to provide an exact independent particle picture of such competition [25].

I have also performed a study on the use of ultrafast field to manipulate nuclear dynamics in molecular devices [26], and provide a general theory based on NEGF on how to describe molecular forces in molecular motors in the presence of interactions [27]. A mixed-quantum

classical scheme along these lines was then introduced to describe skyrmion dynamics, in terms of localized spins and itinerant electrons within NEGF-GKBA [35].

I have also started a line of investigation for time-resolved spectroscopies at surfaces, in terms of explorative models solved exactly [29], via the Kadanoff-Baym equations [31, 32], and in terms of *ab-initio* GW treatments [33]. This has lead also to some work on time dependent spectroscopies for atoms, namely how to affect the Auger decay via the Zeno effect [36].

Finally, generalising previous work, I have studied the dynamical competition of Kondo and RKKY interactions, and how to proceed across different phases in a nonequilibrium Doniach-Phase Diagram [34].

These recent studies, clearly show the necessity of an appropriate treatment of correlations at the *ab initio* level, and for system out of equilibrium. Effort in this direction has just started, with a proposal from our group of an hybrid method which mixes the essential elements of NEGF and TDDFT [37].

## References

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