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PREFACE

Special issue on novel superconducting and magnetic materials

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Preface

Special issue on novel superconducting and magnetic materials

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Superconductivity and magnetism—and their entanglement in a single material—are among the most studied phenomena in condensed matter physics and continue to pose new challenges for fundamental research and exciting opportunities for technological applications. The last decade has witnessed ground-breaking discoveries in both fields: high-temperature superconductivity in compressed hydrides [1–3], unconventional superconductivity in iron-based materials [4, 5] and new types of magnetic states in spin–orbit coupled materials with topological and nematic characteristics [6]. The prediction of material-specific properties and the interpretation of superconducting and magnetic phase transitions have been crucially aided by advances in *ab initio* electronic structure methods within the density functional theory and its extensions [7].

This special issue gathers together selected theoretical and experimental contributions on novel aspects of superconductivity and magnetism, collected in memory of Prof. Sandro Massidda. The collection aims to provide an updated view on timing issues and challenges in this active research field that have been at the hearth of Sandro's scientific interests. As commemorated in the obituary by Continenza and Colombo [8], Sandro has dedicated his scientific work to the development and application of *ab initio* computational and theoretical methods, yet never losing focus to the ultimate goal of theoretical and computational physics, that is to support, complement and understand the experimental observations.

Articles in this issue

This special issues is opened by two viewpoints on the application of first-principles methods for the prediction and interpretation of magnetic and superconducting properties. This approach is nicely introduced by the article by Mazin [9], which offers a reasoned review on how computational schemes to superconductivity have become such essential tools of the field. Igor Mazin highlights the benefit of materials-specific schemes, which are capable to provide a quantitative account of the electronic properties a microscopic level, and identifies in MgB_2 the paradigm shift-point where *band theorists* have established in an incontrovertible way their importance. The following viewpoint addresses one of the long-standing challenge in solid state physics, i.e. room temperature superconductivity [10]. Boeri and Bachelet review the latest achievements of computational superconductivity, singled out in the accurate prediction of nearly-room-temperature superconductivity in high-pressure hydrides.

The next block of contributions report theoretical and methodological developments. Sandro has been one of the driving forces in the development of more and more accurate methods to treat conventional superconductors, such as high-pressure hydrides and MgB_2, where superconductivity is mediated by phonons (lattice vibrations). The contribution by Lüders and coworkers reports methodological advances within the superconducting density functional theory [7], proposing an analytical procedure to efficiently compute the isotope coefficient, a key quantity to decipher the onset of a phonon-mediated superconducting state [11]. In fact, the observation of a finite isotope effect, i.e. a shift of T_C observed upon isotopic substitution, is considered to be the definite 'smoking gun' for conventional superconductivity. The simple BCS theory predicts a standard isotope effect of 0.5, but different values are possible at large couplings or because of anomalous Coulomb effects. The article by Raffaele Resta discusses the nature of Drude and superconducting weights. Both quantities can be extracted by optical experiments, and the author provides a thorough analysis on

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how these two wights can be used to discriminate between insulators, metals, and superconductors [12]. Methodological developments aimed at improving the description of band gap and optical spectra are presented and discuss in the contribution by Wang an coworkers [13], based on an extension of the scissor correction to the domain of real-time linear-response time-dependent density functional theory.

The other contributions in this special issues revolve around applications of first-principles methods to actual magnetic and superconducting materials.

Sandro has loved working on MgB_2, a simple and yet rich system from where a lot of interesting physics has emerged. 18 years after its discovery it still stimulates and offers opportunities for new superconductivity discoveries, such as the one discussed by Ummarino and Romanin [14], of field doping a thin film to improve its superconducting T_C. Moreover, the abundant experimental phenomenology allows for the development of novel interpretative framework. Following this direction, Pallecchi *et al* [15] come up with a rationale to control the Seebeck coefficient by inducing disorder or varying the electron filling of the characteristic π and σ bands of MgB_2. Indirectly, this can provide useful insights on the strength of the electron-phonon coupling.

MgB_2 becomes superconducting at 39 degrees Kelvin, well below room temperature. The discovery of superconductivity in hydrides has demonstrated that it is possible to realize superconductivity close to room temperature, but the pressures involved, of the order of millions of atmospheres, make it unpractical for any real-life application. If one is concerned with realizing room- (or high-) temperature superconductivity at ambient pressure, unconventional superconductors are more likely candidates. The two largest classes of unconventional superconductors, i.e. cuprates, discovered in the late '80 s [16], and iron superconductors, discovered 20 years later [4], have both been central to the work of Sandro. In spite of a great research effort these systems are far from being completely understood. A comprehensive theory is prevented by the occurrence of strong correlations and a complex interplay between a magnetic instability and a pairing induced by subtle magnetic interactions. In spite of the difficulty, it is of vital importance to keep investigating magnetism and superconductivity in Iron- and Copper-based superconductors and in general in strongly correlated systems.

The key role of doping and disorder is reflected in the present collection by several contributions both of computational [17, 18] and experimental type [19–21]. In passing, the effect of doping on superconductivity has attracted also the curiosity of Sandro, see for instance the DFT-based study of Al and Li doping of Mgb_2 [22]. Bernardini's work [17] focuses on the effect of doping in the iron-pnictides. By means of *ab initio* simulations, the authors show that F doping of SmFeAsO has an unexpected behavior; F should be a donor, instead, it behaves as an isoelectronic impurity. This finding suggests the existence of explanations of the origin of superconductivity different from those commonly accepted. The consequences of the substitution of Fe with Mn is addressed in the experimental articles by Sanna *et al* [19] and Martinelli *et al* [20]. The authors show that even a tiny doping level has a strong impact on the structural and magnetic properties and is sufficient to destroy the superconducting state in Fe-based superconductors. A similar suppression of superconductivity has been also reported for the cuprate $YSr_2Cu_3O_{6+x}$ as elaborated in the first principles study of Gauzzi and coworkers [18]. Conversely, combining experiment and DFT, De Renzi and coworkers observe a surprising enhancement of the critical superconducting temperature in $YBa_2Cu_3O_{6+y}$ achieved by hole-doping and disorder, which is associated with an abrupt collapse of the antiferromagnetic ordering temperature. Moving away from the doping effect, the work by Meinero and collaborators study the anisotropy of transport and magnetic properties in the undoped parent superconductor $BaFe_2As_2$, revealing that intrinsic scattering mechanism, possibly combined with electronic correlation effects, is the key ingredient to reach a sound comparison between theory and experiment [23].

The heritage of MgB_2 has been a thriving research on superconductivity in covalent metals, especially those with marked 2D features, such as dichalcogenides and interacalated graphites. Systems that may be potentially interesting for superconductivity are not even limited to those that are metallic at ambient conditions. Metallicity, which is a pre-condition for superconductivity, can in fact be induced in a variety of ways, such as pressure, doping and field effect. Joseph and coworkers [24] discuss on how the application of moderate pressure induces a metal-insulator transition and a complex structural modification in

black-P. The study of [25] shows that the injection of electrons via chemical doping in a 5*d* oxide (oxides are another class of materials largely studied by Sandro using beyond DFT methods, see for instance the seminal work on ZnO [26]) enhances longitudinal spin fluctuations which progressively quench the magnetic band gap. Finally in the Piatti, Romanin and Gonnelli map [27], in a combined experimental-theoretical work that Sandro would have certainly appreciated, the field-induced insulator metal transition in MoS_2.

Other contributions in this issue focus on more general aspects of magnetism in different materials, another topic which was central to Sandro's research interest. Podloucky and Redinger [28] study in detail the stability and magnetic properties of different MnX compounds, and point out severe limitations encountered by standard exchange-correlation functionals in describing these systems. An anomalous magnetic behaviour in the weak antiferrormagnet TiAu upon hole doping is described in [29], reporting a (quantum-)critical coexistence between itinerant and local moments.

The number, variety and quality of the contributions submitted to this special issue testifies the wide reach of Sandro's human and scientific interests. Considering the great effort that Sandro has dedicated to the description of superconducting materials within a full first principles basis, it is our great hope that in a near future parameter-free theoretical simulations for superconductors could be made regardless of the leading pairing interaction. Combined with crystal structure predictions methods and machine learning schemes, as this could speed up the search for new superconducting families similarly to what has been recently done under high pressure for phonon-mediated superconductors. As editors, we would like to thank all the contributors that have accepted to submit their work in this collection. As friends and pupils, we thank Sandro for the joy and passion that he has instilled in us; his teachings, along with his rigorous scientific ethic, will continue to accompany our scientific lives.

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