MM 3: Computational Materials Modelling - Fundamentals

Time: Monday 10:15–11:30 Location: H24

MM 3.1 Mon 10:15 H24

New developments in non-local density functional theory — •Riccardi Sabatini[1,2] and Stefano de Gironcoli[2] — [1]Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne (CH) — [2]Scuola Internazionale Superiore di Studi Avanzati (SISSA), via Bonomea 265, I-34136 Trieste, Italy

Van-der-Waals dispersive interactions are an essential component in the description of soft matter and in many other systems, from metal adsorbates to hydrophobic and hydrophilic interactions. In the last years a great effort has been made within the framework of density-functional theory to overcome the limitations of local or semi-local functionals, and a new class of non-local functionals is now able to take into account dispersive interacitons. We present some of our recent contributions to this field, and some selected applications. In particular, i) we developed and implemented in the Quantum-ESPRESSO distribution a new functional, inspired by the work of Vydrov and Van Voorhis [PRL 103, 06300], that can work very efficiently in a plane-wave basis and shows excellent performance on the reference set S22 of non-covalent complexes, ii) we extended and implemented in density-functional perturbation theory the formalism to treat non-local functionals of the form suggested by Dion et al. [PRL 92, 246401 (2004)], obtaining a simple and efficient way to calculate the vibrational properties of soft materials from first-principles. Finally, we present results on graphite and simple molecules, where these new tools are benchmarked and compared with experimental results or other theoretical approaches.

MM 3.2 Mon 10:30 H24

The physical solution of the *GW* approximation — •Falk Tandetzky, Kay Dewhurst, Sangeeta Sharma, and E.K.U. Gross — Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany

We show[1] that the equations underlying the *GW* approximation have a large number of solutions. To the best of our knowledge no such extra solutions have been reported in the literature yet. This raises the questions: Which is the physical solution? And why do numerical methods converge to it, rather than to one of the spurious solutions? We provide theorems which answer both of these questions. These theorems are general enough to cover a large class of similar algorithms. This fact is important for understanding how vertex corrections can be treated without running into unphysical solutions.

[1] F. Tandetzky, J. K. Dewhurst, S. Sharma, E. K. U. Gross: arXiv:1205.4274

MM 3.3 Mon 10:45 H24

How van der Waals Interactions Influence Cohesive Properties of Solids — •Guo-Xu Zhang, Anthony M. Reilly, Alexandre Tkatchenko, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin, Germany

Standard semilocal and hybrid density functionals are widely used for studying cohesive properties of many covalent, metallic, and ionic materials. Only recently it has been recognized that long-range van der Waals (vdW) interactions, that are missing in all semilocal and hybrid functionals, are important for an accurate description of cohesion in solids. Here we construct a database of 64 solids where reference cohesive properties are obtained from a critical revision of the available experimental data. All-electron DFT calculations with explicit treatment of zero-point vibrations for all cohesive properties are carried out using the local-density approximation (LDA), Perdew-Burke-Ernzerhof (PBE) GGA, and the empirical meta-GGA M06-L [1] functionals. For 23 semiconductor solids, we also carry out PBE and M06-L calculations with the inclusion of fully screened long-range vdW energy [2]. We find that PBE is the most systematic from the three employed functionals, and its accuracy is improved by a factor of two after the inclusion of vdW interactions. The LDA functional considerably overbinds for all the studied solids. The M06-L functional describes middle-range correlation better for certain semiconductors and ionic crystals, but fails for heavier semiconductors and metals. [1] Zhao and Truhlar, JCP (2006). [2] Tkatchenko, DiStasio, Car, Scheffler, PRL (2012).

MM 3.4 Mon 11:00 H24

The importance of many-body dispersion interactions for molecular materials — •Anthony Reilly and Alexandre Tkatchenko — Fritz-Haber-Institut der MPG, Berlin, Germany

It is now well established that dispersion interactions are essential to the stability and properties of soft-matter and molecular materials. However, many computational approaches use simple pairwise approximations to include these interactions, ignoring their origin in collective many-body plasmonic excitations. Using the recently developed many-body dispersion (MBD) method (PRL 108, 236402; PNAS 109, 14791) and a database of molecular-crystal structures, we show that a realistic many-body treatment of dispersion interactions has a significant impact on molecular-crystal stability. Crucially, coupling the MBD method with DFT calculations allows *ab initio* modelling to reach within the highly coveted "chemical accuracy" with respect to experimental enthalpies of sublimation. The results show that the accurate modelling and prediction of molecular materials necessitates an accurate and "beyond pairwise" treatment for dispersion interactions.

MM 3.5 Mon 11:15 H24

Metamaterials and cosmological inflation — •Grigoris Panotopoulos and Keshav Dani — Femtosecond Spectroscopy Unit, Okinawa Institute of Science and Technology, Graduate University, Okinawa, Japan

Inflation is widely accepted to be the best paradigm we have today for the physics of the early universe. It solves the lond-standing problems of hot big-bang cosmology, and at the same time it generates the primordial fluctuations responsible for the structures we observe in the universe today. On the other hand, metamaterials are laboratory made, artificial materials with new exotic properties not found in other substances in nature, and they can have numerous interesting applications. In the present work we make a connection between hyberbolic metamaterials and cosmological inflation. We show that if the permittivities of the metamaterial are appropriately chosen, then the Maxwell's equation for the light propagation in the sample matches the equation for the metric perturbation, and for a concrete inflationary model we find exact analytical solutions. Therefore, not only can inflation be reproduced in the laboratories, which is interesting on its own, especially now that the Planck mission is taking data and may see gravitational waves as predicted from inflation, we may also obtain interesting solutions for the electric field in the metamaterial (Bessel functions), based upon cosmological solutions.