

MM 27: Computational Materials Modelling - Electronic structure approaches

Time: Tuesday 10:15–11:15

Location: IFW B

MM 27.1 Tue 10:15 IFW B

A Compressed-Sensing Approach to Select Accurate Atom-Centered Basis Functions for Advanced Density Functionals and Quantum Chemistry — •NIKLAS MENZEL¹, LUCA M. GHIRINGHELLI¹, GITTA KUTYNIOK², and MATTHIAS SCHEFFLER^{1,3} — ¹Fritz-Haber-Institut der MPG, Berlin, DE — ²Technische Universität, Berlin, DE — ³UC Santa Barbara, USA

The choice of basis sets is a crucial factor in density functional theory and quantum chemistry, determining the accuracy and computational cost of the calculation. Commonly used basis sets are not sufficiently accurate to represent the eigenfunctions for advanced exchange-correlation treatments. This leads to basis set extensions, such as the correlation-consistent basis sets by Dunning [JCP 90, 1007 (1989)]. We have developed a new approach to select basis functions based on compressed sensing (CS), a recently developed signal processing technique. CS provides a simple and efficient framework for basis set selection based on ℓ_1 -norm regularization. Our CS-based approach is applicable to all atom-centered basis sets. As introductory example, we demonstrate the selection of Gaussian-type basis functions (GTO). The number of chosen contracted or uncontracted GTOs can be tuned. We calculate the total energy for atoms from H to Ar and compare the results with Dunning's correlation-consistent basis sets, which give similar results. Our new approach enables us to determine accurate basis sets for heavier atoms including d - and f -elements.

MM 27.2 Tue 10:30 IFW B

High-order path integrals made easy — •VENKAT KAPIL¹, JÖRG BEHLER², and MICHELE CERIOTTI¹ — ¹Laboratory of Computational Science and Modelling, Institute of Materials, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — ²Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, Bochum, Germany

The precise description of quantum nuclear fluctuations in atomistic modelling is possible by employing path integral techniques, which involve a considerable computational overhead due to the need of simulating multiple replicas of the system. Many approaches have been suggested to reduce the required number of replicas. Among these, high-order factorization of the Boltzmann operator are particularly attractive for high-precision and low-temperature scenarios. Unfortunately, to date several technical challenges have prevented a widespread use of these approaches to study nuclear quantum effects in condensed-phase systems. Here we introduce an inexpensive molecular dynamics scheme that overcomes these limitations, thus making it possible to exploit the improved convergence of high-order path integrals without having to sacrifice the stability, convenience and flexibility of conventional second-order techniques. The capabilities of the method are demonstrated by simulations of liquid water and ice, as described by a

neural-network potential fitted to dispersion-corrected hybrid density functional theory calculations.

MM 27.3 Tue 10:45 IFW B

New Dynamical Mean-Field Theory capabilities in CASTEP — •EVGENY PLEKHANOV¹, VINCENT SACKSTEDER², PHIL HASNIP³, MATT PROBERT³, STEWART CLARK⁴, CEDRIC WEBER¹, and KEITH REFSON² — ¹Department of Physics, Faculty of Natural and Mathematical Sciences King's College London Strand, London, WC2R 2LS, UK — ²Department of Physics, Royal Holloway University of London, Egham, Surrey TW20 0EX, UK — ³Department of Physics, University of York, Heslington, York YO10 5DD, UK — ⁴Department of Physics, University of Durham, Durham DH1 3LE, UK

We present the first implementation of Dynamical Mean-Field Theory in UK's major ab-initio code CASTEP [1]. This implementation: i) is modular; ii) allows great flexibility in choosing local basis set for downfolding/upfolding of self-energy; iii) permits wide choice of impurity solvers (including external solver libraries); and iv) gives the user a possibility to use several self-consistency schemes and calculate total energy and forces. We explain in details the theoretical framework used. We benchmark our implementation on several strongly-correlated insulating systems with d - and f -shells: γ -Ce and Ce_2O_3 by using Hubbard I and CTHYB-QMC solvers. Our results appear to be in excellent agreement with the reference data published previously in the literature [2,3,4].

[1] E. Plekhanov, et al. in preparation (2016). [2] L. Pourovskii, et al. Phys. Rev. B 76, 235101 (2007). [3] B. Amadon, et al. Phys. Rev. B 77, 205112 (2008). [4] J. Kuneš, et al. Phys. Rev. Lett. 99, 156404 (2007).

MM 27.4 Tue 11:00 IFW B

Analytical continuation of Green's functions using Padé approximants — •JOHAN SCHOTT — Uppsala University, Uppsala, Sweden

A critical step to obtain physical observables for many Green's function based methods is the ill-posed analytical continuation problem. We propose to remedy the known instability problems of the Padé approximant method by averaging several continuations, using different number of Padé approximant coefficients and input points. In our article [Phys. Rev. B 93, 075104 (2016)] we also show including negative Matsubara frequencies further improves the peak resolution possibility. The importance of high numerical precision, even for very noisy input data, is systematically presented. Lastly, the presented method is compared to a number of other analytical continuation methods, showing good performance.