Réunions scientifiques

Séminaires

Séminaire SOLEIL

First-principles description of correlation : from simple metals to oxides

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Invité par Fausto SIROTTI

Methods based on Green's functions, like the GW approximation or the Bethe-Salpeter equation (BSE), are powerful tools in unveiling new physics, as we also have recently shown for dense sodium [1] (a charge-transfer insulator at high pressures) and solid picene [2] (a first example of a new class of organic superconducting materials). Here we show how the application of first-principles GW and BSE can be further extended towards more strongly correlated materials, at the example of the metal-insulator transition (MIT) in vanadium dioxide [3]. We prove that i) ab initio GW provides a consistent interpretation of the transfer of spectral weight across the MIT in the photoemission spectra, not only for V d states close to the Fermi energy, but also for V s states at higher binding energies [4]; ii) excitonic and crystal local-field effects are important for the interpretation of optical spectra in the insulating phase and can be adequately described by the BSE [5]. We further discuss the limitations of the methods and their applications to other correlated transition-metal oxides.

Work done in collaboration with P. Cudazzo, I. Tokatly, and A. Rubio (ETSF – UPV San Sebastian, Spain), F. Iori, M. Guzzo, R. Hambach, F. Sottile, and L. Reining (ETSF - LSI Ecole Polytechnique Palaiseau, France), F. Bruneval (CEA Saclay, France), V. Olevano (CNRS Grenoble, France), G. Panaccione (TASC Trieste, Italy), F. Offi (Uni. Roma 3, Italy), M. Marsi (LPS Orsay, France), F. Rodolakis and J.-P. Rueff (Synchrotron Soleil, France), and M. Knupfer (IFW Dresden, Germany).

References

[1] M. Gatti, I.V. Tokatly, and A. Rubio, Sodium: a charge-transfer insulator at high pressures, Phys. Rev. Lett. 104, 216404 (2010).
[2] F. Roth, M. Gatti, P. Cudazzo, M. Grobosch, B. Mahns, B. Büchner, A. Rubio, and M. Knupfer, Electronic properties of molecular solids: the peculiar case of solid picene, submitted.
[3] M. Gatti, F. Bruneval, V. Olevano, and L. Reining, Understanding correlations in vanadium dioxide from first principles, Phys. Rev. Lett. 99, 266402 (2007).
[4] E. Papalazarou, M. Gatti, M. Marsi, V. Brouet, F. Iori, L. Reining, E. Annese, I. Vobornik, F. Offi, A. Fondacaro, S. Huotari, P. Lacovig, O. Tjernberg, N. B. Brookes, M. Sacchi, P. Metcalf, and G. Panaccione, Valence-band electronic structure of V2O3: Identification of V and O bands, Phys. Rev. B 80, 155115 (2009).
[5] M. Gatti, F. Sottile, and L. Reining, in preparation.

Formalités d'entrée *: accès libre dans l'amphi du Pavillon d'Accueil. Si la manifestation a lieu dans le Grand Amphi Soleil du Bâtiment Central, merci de vous munir d'une pièce d'identité (à échanger à l'accueil contre un badge d'accès).*

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