Coupling of excitations in electronic spectra: fingerprints of correlation

Lucia Reining

Laboratoire des Solides Irradiés, CNRS, Ecole Polytechnique, 91128 Palaiseau, France

Electronic excitations determine the characteristics of materials all over science and technology, from photochemistry to radiation defects, from synchrotron experiments to cancer research. Theory and numerical modelling are valuable tools for the understanding and prediction of many of the important phenomena. During the last decades, the field has evolved rapidly. In particular, it is today possible to calculate optical spectra ab initio, i.e., without ajustable parameters, including the correlation between electron and hole [1]. Numerous conceptual and technical problems had to be solved to reach this aim, and much remains to be done. For example, the question of how to include the description of satellite structures, that derive from coupling between excitations, is a topic of current research [2].
This talk will give an overview of the state-of-the art in ab initio calculations of optical spectra of materials, focussing on the main ideas of the underlying theories, their conceptual and technical limitations, and useful comparisons with, and interpretation of, experiment. It will also contain a glance at the most recent developments as well as the challenges that modern experiments and technological needs put forward to theory. Systems used for illustration will include models, semiconductors, and carbon structures.
Throughout this talk the outstanding contributions of Rodolfo Del Sole will be highlighted, who has been a key person in moving the field forward [3].

References

[1] see e.g. G. Onida, L. Reining. R.W. Godby, R. Del Sole and W. Andreoni, Phys. Rev. Lett. 75, 818 (1995); S. Albrecht, L. Reining, R. Del Sole, and G. Onida, Phys. Rev. Lett. 80, 4510 (1998).
[2] M. Guzzo, G. Lani, F. Sottile, P. Romaniello, M. Gatti, J.J. Kas, J.J. Rehr, M.G. Silly, F. Sirotti, and L. Reining, Phys. Rev. Lett. 107, 166401 (2011).
[3] M. Palummo, G. Onida and L. Reining, *In memoriam of Professor Rodolfo Del Sole Obituary,* Phys. Stat. Solidi (b) 249, 1092 (2012).

**corresponding author: lucia.reining@polytechnique.fr*