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# EINLADUNG zum IFP-SEMINAR

## *GW* and post-*GW* calculations for molecular systems

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| Host: | Jan Tomczak, Karsten Held |
| Termin: | Montag, 12 Juni 2017, 10:30 Uhr |
| Ort: | Institut für Festkörperphysik, TU Wien |
| | Wiedner Hauptstraße 8-10, 1040 Wien |
| | Seminarraum DB gelb 09 (gelber Bereich, 9. OG) |

Hedin's breakthrough in many-body physics is a computationally man-ageable scheme [1] to implicitly account for many-body effects thanks to the introduction of a self-energy, whose expression is known but in practice approximated by truncation at some order in the inter-particle interaction.

Hedin's scheme allows the computation of quasi-particle addition and removal energies. The introduction of an added particle (or hole) to the system will trigger the formation of higher order neutral excitations (particle/hole pairs formation). The widespread *GW* approximation only partially accounts for these effects by replacing the bare interparticle interaction with a dressed one. Other correlation effects are contained in the vertex function [2] and are typically disregarded.

In this talk, the performance of the *GW* approximation is assessed for a large set of molecules [3]. Furthermore, Hedin's scheme is solved with the inclusion of the vertex function (*GW*Γ). This computational scheme allows for the consistent inclusion of the vertex both at the polarisability level and in the self-energy. The latter is related to the kernel of the Bethe-Salpeter equation and to the corresponding polarisation propagator. The inclusion of the vertex produces very satisfactory agreement with experimental removal energies and wavefunction-based results.

[1] L. Hedin, Phys. Rev. **139**, A796 (1965).
[2] G. Strinati, La Riv. del Nuovo Cim. **11**, 1 (1988).
[3] E. Maggio, P. Liu, M. J. van Setten, and G. Kresse, J. Chem. Theory Comput. **13**, 635 (2017).