



ID de Contribution: 242

Type: Poster

## Electron removal energies in noble gas atoms up to 100 keV: *ab initio* GW vs XPS

mardi 21 mars 2023 17:30 (1h 30m)

X-ray photoelectron spectroscopy (XPS) measures electron removal (quasiparticle) energies, providing direct access to core and valence electron binding energies, hence probing the electronic structure. We present the benchmark of the *ab initio* many-body *GW* approximation on the complete electron binding energies of noble gas atoms (He-Rn), which spans 100 keV. Our results demonstrate that *GW* achieves an accuracy within 1.2% in XPS binding energies, by systematically restoring the underestimation from density-functional theory (DFT, error of 14%) or the overestimation from Hartree-Fock (HF, error of 4.7%). Such results also imply the correlations of *d* electrons are very well described by *GW*.

**Auteurs principaux:** M. MUKATAYEV, Iskander (UGA, CEA-Leti); Dr SKLÉNARD, Benoît (CEA-Leti, UGA); OLEVANO, Valerio (CNRS, Institut NEEL); Dr LI, Jing (CEA-Leti, UGA)

**Orateur:** OLEVANO, Valerio (CNRS, Institut NEEL)

**Classification de Session:** Cocktail & Poster session

**Classification de thématique:** Many-body