UNIVERSITÄT DUISBURG ESSEN

Offen im Denken

Theorie-Kolloquium WS 2024/25
Fr 24.01.2025, 14:00-15:30
Online (URL in E-Mail)

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Prediction of deep core-level spectra of large systems with *GW* and beyond

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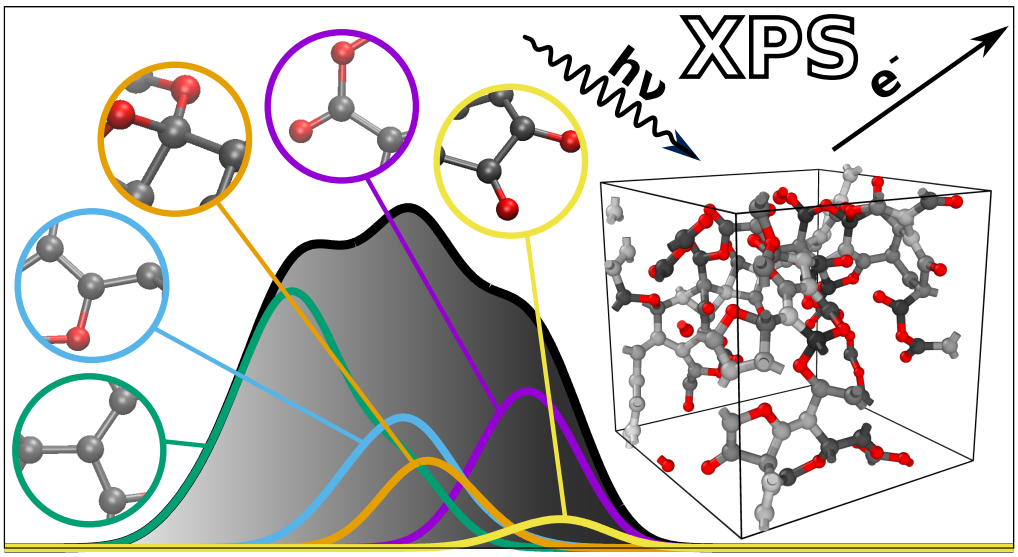

Figure: Core-electron binding energies in carbon-based materials: A machine-learning model combining density-functional theory and GW [4].

While the *GW* method is well-established for calculating valence photoemission spectra of solids and molecules [1], its application to deep core levels with excitation energies exceeding 100 eV is a more recent advancement. Core-level spectroscopy, which probes the local atomic environment without constraints on symmetry or periodicity, serves as a powerful technique for chemical analysis and materials characterization. We have demonstrated that *GW* yields accurate absolute and relative 1s core-level binding energies, with deviations of 0.3 eV and 0.2 eV from experimental values, respectively [2].
This talk covers our recent efforts to extend computations to: i) large systems and ii) shake-up satellites. For large systems, we focus on implementing low-scaling algorithms [3] combined with machine learning approaches [4]. For shake-up satellites, we explore the application of vertex corrections [5].

[1] D. Golze, M. Dvorak, and P. Rinke. Front. Chem., 7:377, 2019.
[2] D. Golze, L. Keller, and P. Rinke. J. Phys. Chem., 11:1840, 2020.
[3] R. L. Panadés-Barrueta and D. Golze. J. Chem. Theory Comput., 19:5450, 2023.
[4] D. Golze, M. Hirvensalo, P. Hernández-León, A. Aarva, J. Etula, T. Susi, P. Rinke, T. Laurila, and M. A.. Caro. Chem. Mater., 34(14):6240, 2022.
[5] J. Kockläuner and D. Golze. arXiv:2412.17132, 2024.