Absolute Binding Energies of Core Levels in Solids from First Principles

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The X-ray photoelectron spectroscopy (XPS) is one of the most important and widely used techniques in studying chemical composition and electronic states in the vicinity of surfaces of materials. In spite of the long history of XPS and its importance in materials science, a general method has not been developed so far to calculate absolute binding energies for both insulators and metals, including multiple splittings due to chemical shift, spin-orbit coupling, and exchange interaction, on equal footing. Here, we propose a general method to calculate absolute binding energies of core levels in metals and insulators, based on a penalty functional and an exact Coulomb cutoff method in a framework of the density functional theory [1]. It is demonstrated that the absolute binding energies of core levels for both metals and insulators are calculated by the proposed method in a mean absolute (relative) error of 0.4 eV (0.16 %) for eight cases compared to experimental values measured with XPS within a generalized gradient approximation to the exchange-correlation functional. Recent applications of the method including silicene [2], borophene, and platinum atoms will also be discussed in comparison with experimental data..

Bibliography

[1] T. Ozaki and C.-C. Lee, Phys. Rev. Lett. 118, 026401 (2017).
[2] C.-C. Lee et al., Phys. Rev. B 95, 115437 (2017).

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http://www.openmx-square.org/