



Soutenance HDR

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Theoretical spectroscopy: from periodic systems to isolated nano-objects

This presentation for my Habilitation à Diriger des Recherches provides a non-exhaustive summary of my scientific career. Following an initial period as an experimentalist at the French National Synchrotron (LURE), I transitioned toward theoretical spectroscopy by joining the Laboratoire des Solides Irradiés. My research has since focused on the study of low-dimensional systems using *ab initio* formalisms, such as Time-Dependent Density Functional Theory (TDDFT), to account for local field effects. Through a fruitful collaboration, I developed a framework to circumvent the limitations inherent in the supercell approach within reciprocal-space codes. During the most recent PhD thesis I supervised, we demonstrated that the TDDFT formalism derived for three-dimensional materials — specifically the Adler-Wiser formula and the identity of longitudinal and transverse dielectric functions in the optical limit — is not valid for 2D objects. By incorporating a proper definition of the 2D layer thickness, we demonstrated that the calculated observable is the transmittance, which simultaneously captures both absorption and plasma resonances. These unexpected results were subsequently confirmed by experimental measurements of the transmittance of a WS₂ monolayer.

