

From structure to opto-electronic excitations of organic-inorganic hybrid materials: State of the art and challenges

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Organic-inorganic hybrid materials are most exciting in view of applications in optoelectronic applications as one can expect to find new properties, which are absent in either of the building blocks. At the same time, they represent challenges for electronic-structure theory as non-local exchange and correlation effects are crucial on all levels, from structure to electronic structure and opto-electronic excitations. Moreover, methods that turned out useful for describing one side may not be applicable for the other one, and they are likely to fail for the interfaces. I will present selected examples of hybrid interfaces to discuss which properties can be reliably computed for such materials and what is missing in our theoretical concepts to reach predictive power on a quantitative level. They will cover photoemission spectra computed by the *GW* approach as well as optical properties including excitonic effects as obtained from the Bethe-Salpeter equation of manybody perturbation theory.