Effect of the chemical composition and dimensionality of halide perovskites for photovoltaic applications on their basic properties: Towards a stable perovskite

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The chemical compositions and dimensionality (3D (bulk), 2D (surfaces, interfaces, thin films) and 0D (nanorod)) of materials for photovoltaic applications strongly influence the performances of solar cells. Their impact concerns mainly the electronic properties and the domains and surfaces stabilities of the different compounds. In the photovoltaic domain, hybrid organic inorganic halide perovskite solar cells have achieved certified record efficiencies over 26%, and tandem cell efficiencies greater than 33%. Though they have displayed dramatic advances; their instabilities against light, heat, and moisture[1] remains a technological lock for their industrial and societal application. Recently emerged fully inorganic perovskites have already demonstrated efficiencies up to 21%, with improved stability. However, these materials have rich sequences of phase transitions associated in particular to the existence of soft phonon modes which can nevertheless still locally generate phase instabilities.
Considering the example of certain organic and inorganic perovskites, this presentation aims to illustrate how their phase transitions, chemical compositions and dimensionality (surface effects) influence their physical and chemical properties and impact the performance of a corresponding perovskite solar cell.

This work is based on a multiscale approach which couples atomistic scale first-principles calculations to device scale numerical models.
At the first-principles level, the evolution of the electronic, vibrational, and dielectric properties of each perovskite is systematically investigated, using a hybrid exchange-correlation functional optimized to yield description of their structural, electronic, and phonon properties, in good agreement with experiment[2]. The influence of the different ions on their phase stability, and, on the insertion and adsorption of H_2O, CO, CO_2 and O_2 in the bulk materials and on various surfaces[3] is analyzed in terms of phonon mode dynamic, optoelectronic and structural properties of the materials.
The resulting band gaps, work functions and dielectric responses serve as input data to the device model which yields the performance of solar cells. This multiscale approach allows to provide a set of criteria for optimizing the materials for different PV applications and for suggesting effective complex perovskites.

REFERENCES

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