Quantum Mechanical Evaluation of New Solar Energy Conversion Materials

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We have launched a major research effort to use quantum mechanics techniques to search for robust, efficient, and inexpensive new materials for photovoltaics (PVs) that convert sunlight to electricity and photo-catalytic electrodes (PCEs) that convert sunlight, carbon dioxide, and water into fuels. Various observables that are key metrics for determining the utility of a given material can be accurately calculated from quantum mechanics; we will discuss our theoretical schemes for each observable and how we validate our approach. The cost-efficiency tradeoff for PV materials based on ultrapure silicon or tandem semiconductor cells motivates a look at new options, and despite periodic media reports to the contrary, no efficient PCEs are available yet. I will discuss why it is so difficult to find effective PCE materials; in particular I will enumerate the very significant constraints beyond those on PVs that they must satisfy to achieve high efficiency. Limiting oneself to abundant elements further constrains the design space. As a result, we are focusing primarily on first row transition metal oxide parent materials, suitably doped or alloyed with other abundant elements. Key material properties, along with some new design principles, will be discussed. The work is revealing which dopants or mixed oxides are most likely to provide solar energy conversion materials that optimize the cost-performance tradeoff.

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