Computational prediction of materials for the sustainable production and storage of energy

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Abstract: Energy sustainability is a vital challenge for humanity. Solving this question requires materials able to convert and store energy efficiently. The *Materials Optimization and Simulation by Ab Initio Computation* (MOSAIC) group develops robust computational tools to understand, predict and optimize the materials for energy conversion and storage and for energy-efficient technologies, such as photovoltaics, (photo)electrocatalytic cells, electrocaloric cooling systems, and next-generation microelectronics. In MOSAIC, we employ electronic-structure methods, embedding approaches, and data-driven inference to accelerate the discovery of these materials, working closely with experimental groups. Examples of research activities outlined in this poster include the computational modeling of ferroelectric thin films for low-power microelectronic memories and switches, of photocatalysts and electrocatalysts for hydrogen production and use, and of defect-tolerant semiconductors for solar energy conversion.