Science of hydrogenated *a*-silicon and its application to photovoltaic devices

Hydrogenated amorphous silicon (*a*-Si:H) is one of the most important energy-storage materials that can convert photovoltaic (PV) energy, using *a*-Si:H-based solar cells or PV modules. However, the efficiency, stability and durability of *a*-Si:H-based solar cells or PV modules largely depend on the microstructural and optoelectronic properties of *a*-Si:H. A major goal of our project is to address the role of microstructural distribution of hydrogen and voids in *a*-Si:H and a quantitative description of these inhomogeneities in *a*-Si:H. Nuclear magnetic resonance (NMR), calorimetry and infrared (IR) experiments indicate that hydrogen atoms bonded to silicon atoms on the void surfaces can desorb to form H_2 molecules. The formation of H_2 molecules introduces dangling or weak Si-Si bonds on the void surfaces, which produce defect states that adversely affect the electronic and optical properties of the material. However, a direct first-principles study of voids on the nanometer length scale has not been possible up until recently because of the lack of appropriate simulation methods that can produce structural models with a linear dimension of several tens of nanometer. We addressed this problem by developing new methodologies, as described under metadynamics, and produced, for the first time to our knowledge, a distribution of voids in *a*-Si:H on the nanometer length scale.