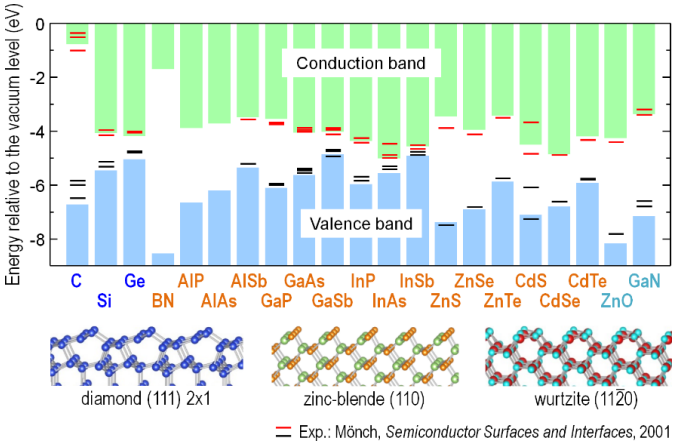
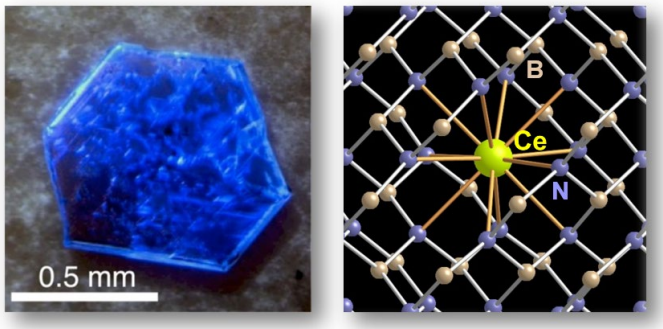
Design and exploration of electronic and energy materials based on computational science

With remarkable developments in computational science and the performance of supercomputers, first-principles calculations now allow us to better understand materials on the atomistic and electronic levels. Furthermore, accurate predictions can be made on the formation of as-yet-unknown materials and their potential functionalities. We utilize cutting edge computational science to discover novel materials with outstanding properties, while also prioritizing cost, environmental friendliness, and elemental abundance. Our research targets include a wide variety of electronic and energy materials for applications such as electronic devices and photovoltaic cells.



Band alignment of semiconductors at their surfaces. Experimental band positions are well reproduced by accurate first-principles calculations, implying that reliable theoretical predictions can be made for experimentally as-yet-uncharacterized materials as well as known materials.



Blue luminous centers in a Ce-doped BN single crystal: A cathodoluminescence image (left) and the local structure of a Ce impurity-B vacancy complex predicted using first-principles calculations (right). Ce impurities have a huge size mismatch with the host B and N atoms. Nevertheless, they can be incorporated into the BN crystal via forming the defect complex involving a Ce impurity and four B vacancies and thereby compensating the mismatch.