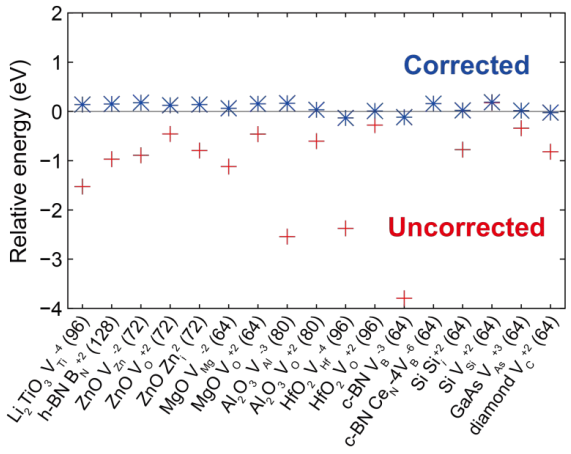
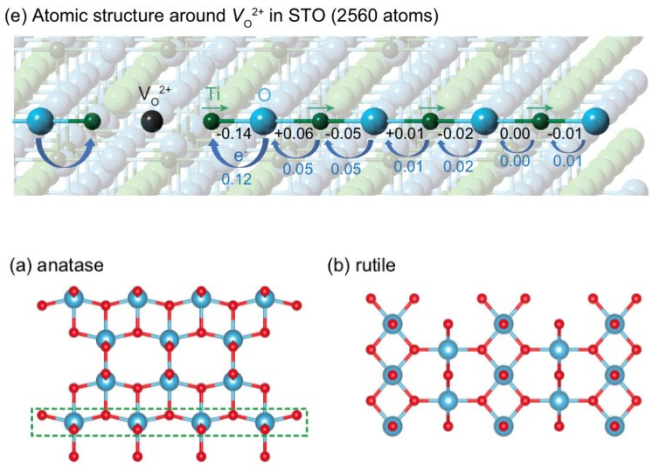
Design and exploration of electronic and energy materials based on computational science

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.



Errors of the defect formation energies in various materials caused by utilizing finite-size supercells. One can see, when using our correction methods, the formation energies are accurately calculated. This method is now recognized by other researches as a versatile correction method.



One-dimensionally extended oxygen vacancy state in strontium titanate predicted by first-principles calculations. Such extended state is found to emerge when a material has large Born effective charges and one-dimensional structural feature. Our finding also explains the reason why the oxygen vacancy shows shallow states in anatase TiO_2 but deep ones in rutile counterpart.