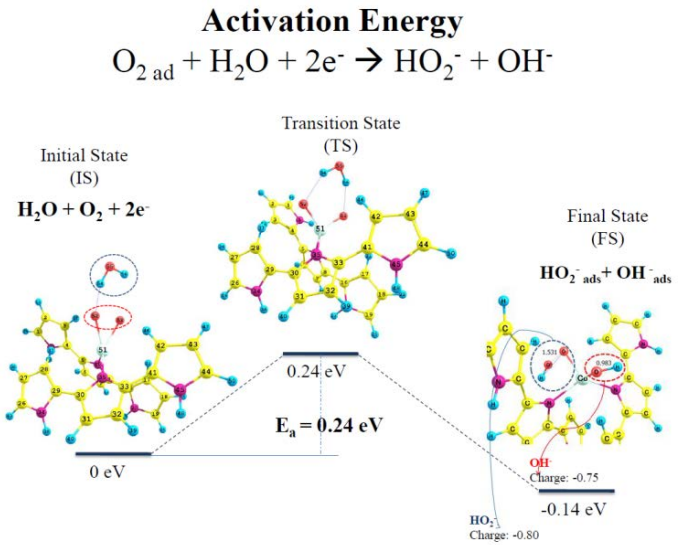
Investigation and design of novel material properties from quantum first-principles calculations

大阪大学工学部・工学研究科・笠井研究室

- ✓ Theoretical study of dynamics and characteristics of materials by quantum first-principles calculations (Density Functional Theory, Quantum Monte Carlo etc).
- ✓ Design of material with novel properties.

Theoretical study based on first-principles calculation have been done on various types of materials. Materials with property related to the green energy applications, electronic and spintronic devices have been investigated. For the energy applications, the research focus is the physical and chemical properties of catalytic reaction on fuel-cell electrodes. Attentions have been given into the electronic structure such as d-band center, magnetic effect etc, to the reaction of molecule with metal, alloy, oxide and polymer & macrocyclic material.

Investigation on materials properties relevant to electronic and spintronic applications have been done and mainly focusing on oxide material for memory device and systems with strongly-correlated electronic properties.



利用者氏名:
笠井 秀明, Wahyu Tri Cahyanto, Nguyen Tien Quang, Eben Sy Dy, Agusta Mohammad Kemal, Kuncoro Handoko Setyo, Hghiem Hoa Thi Minh, 岡 耕平, Febdian Ryusydi, Alaydrus Musa, 岸 浩史