

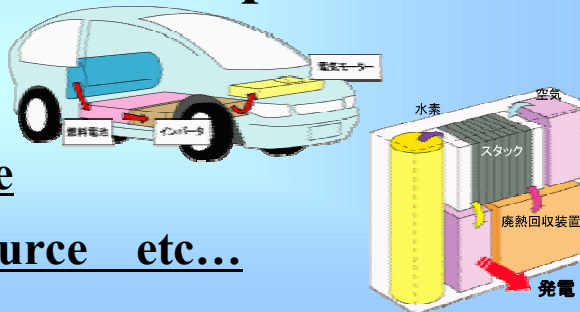
	PEFC	PAFC	MCFC	
electrolyte	polymer	phosphoric acid	fused carbonate	
operating temperature (°C)	below 100	200	600~700	
fuel	H ₂	H ₂	H ₂ , CO	
generating efficiency (%)	30~40	35~45	45~55	
generating scale	small	medium	large	large

Electric generation of small and medium scale is hoped.

dispersed power source

auxiliary power on vehicle

household small power source etc...



Advantage

- simple system
- heat and chemical stability

We want to take advantage of SOFC's feature by sending down operating temperature.

How do we send down
operating temperature?

Improvement in the anode
performance is important.

Purpose of this work

Analysis of hydrogen reaction
by using simulation



Optimal design of anode

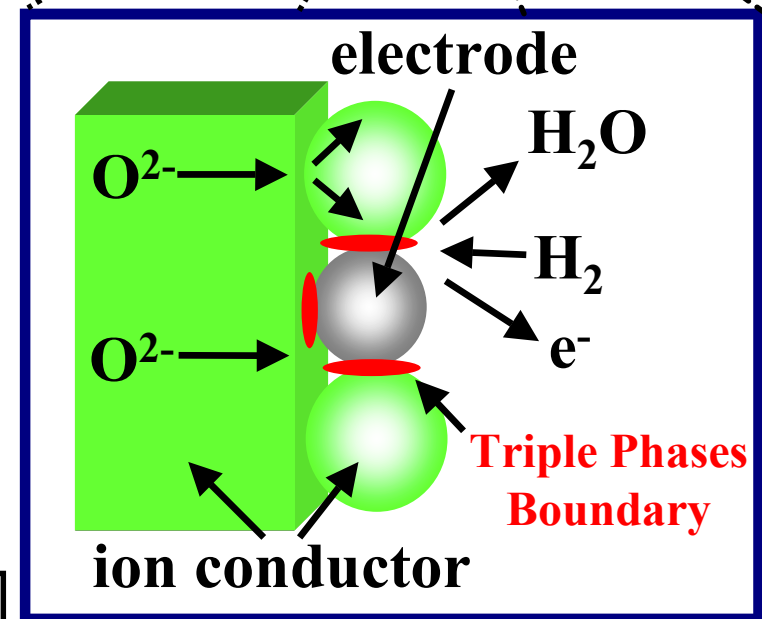
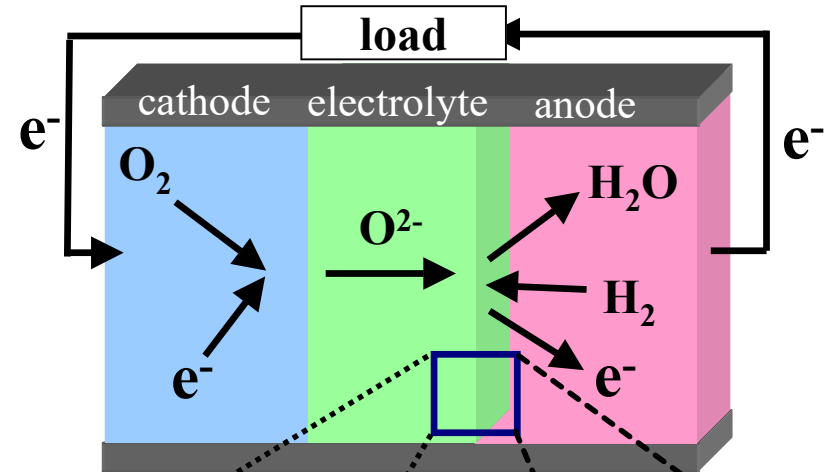
Model construction



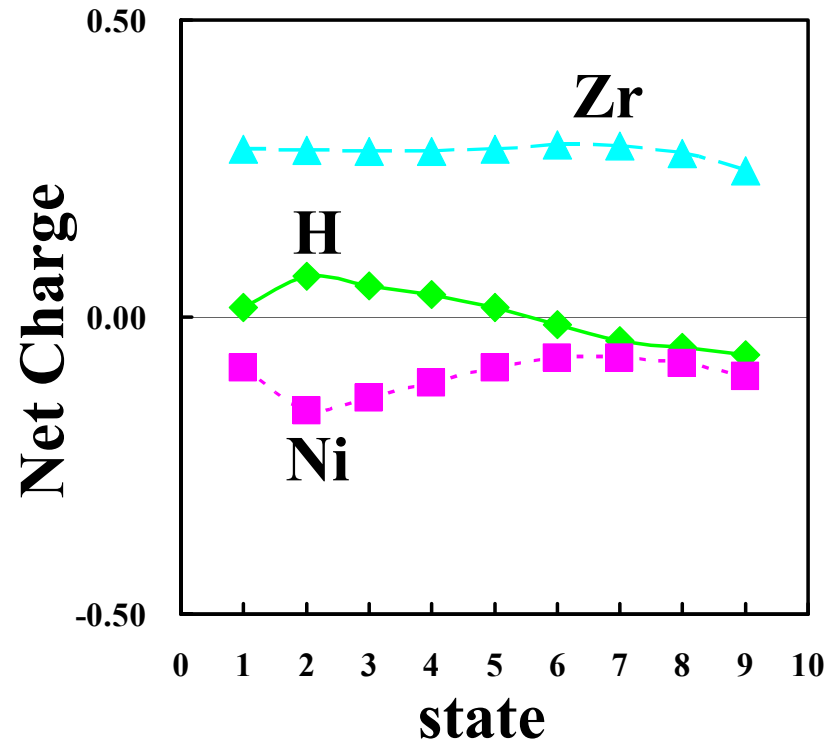
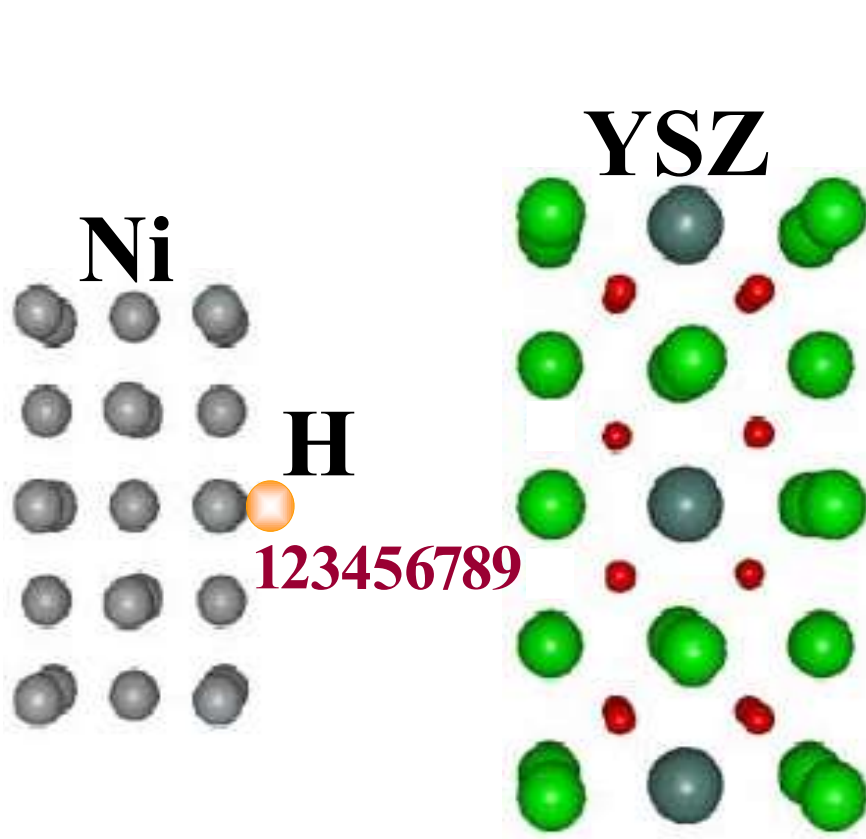
Reactivity assessment

Molecular
dynamics

Quantum chemical
calculation



Electronic state of Ni-YSZ boundary



charge transfer of H, Ni, Zr atom at each state in Ni-YSZ boundary

State 1-6 : Electron transfer between Ni and H.

Maximum value of H valence in state 2.

State 7-9 : Electron transfer between Zr and H.

**Electronic interaction is strong between Ni and H.
Hydrogen reaction is activated in vicinity of state 2.**