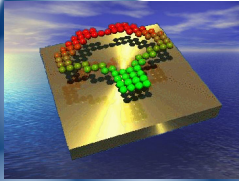


The 3rd Workshop on Environment and Energy (WEE2006)

Hydrogen Energy and Fuel Cells

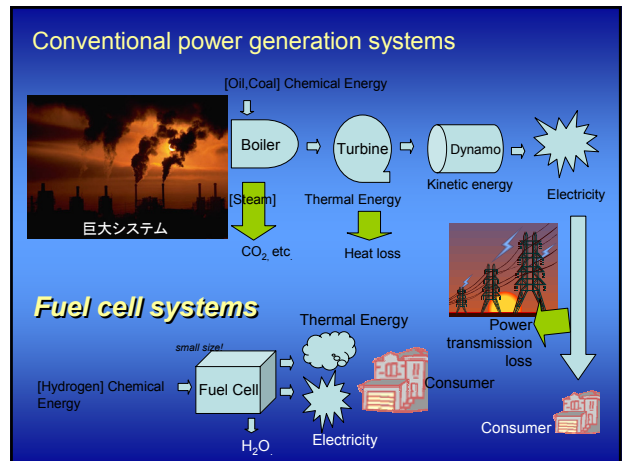
水素エネルギーと燃料電池



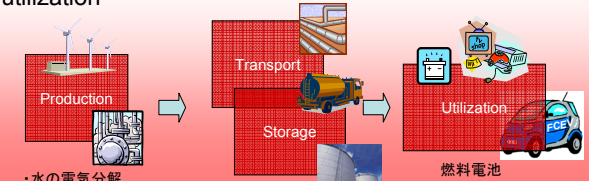
Hideaki Kasai and Tanglaw Roman

Department of Precision Science & Technology and Applied Physics, Graduate School of Engineering, Osaka University

www.dyn.ap.eng.osaka-u.ac.jp



Problems in hydrogen production, transportation, and utilization



Production

- 水の電気分解
- 太陽光発電
- 風力発電
- 核融合...他
- 燃料改質
- 有機燃料 (アルコール、天然ガス...)
- Q. 再生産可能なエネルギー源、

Transport

- ガス
- ボンベ、パイプライン
- 液化水素
- 水素吸蔵物質
- 改質前燃料で輸送
- 消費地で改質
- Q. 安全性、効率


Utilization

- 燃料電池
- Q. 安全性
- Q. 耐久性
- Q. 材料 資源
- Pt: プラチナ
- Pd: パラジウム

Materials analysis and design: the computational approach

物質の性質を探求する学問


前進するための両輪



コンピュータの発達

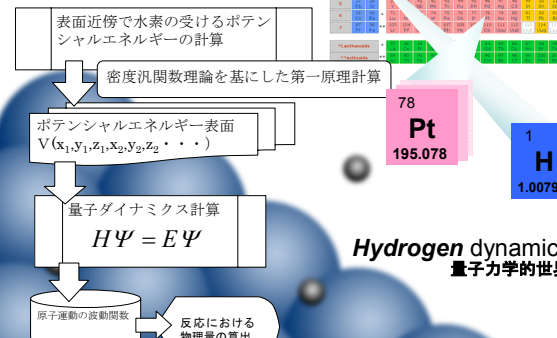
コンピュータの中で、原子の振る舞いを計算シミュレーション(模擬実験)

物質をデザイン



First Principles Calculations

経験的パラメータを排除



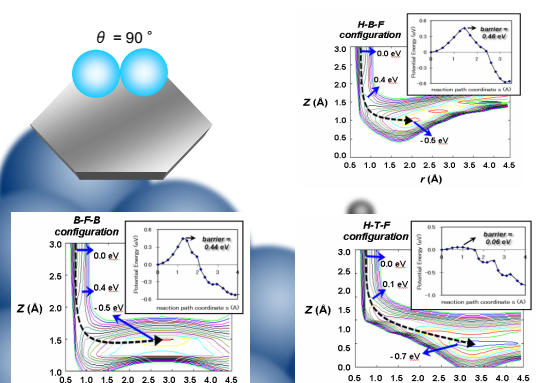
78 Pt 195.078

1 H 1.00794

Hydrogen dynamics 量子力学的世界

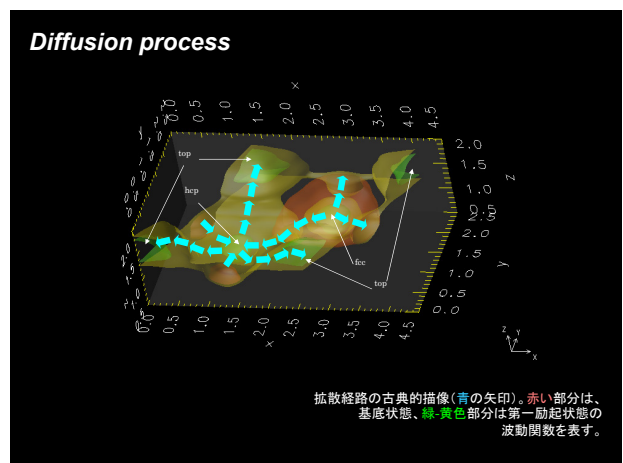
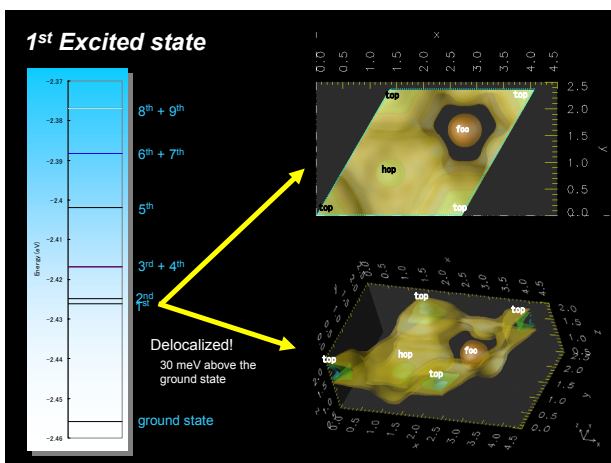
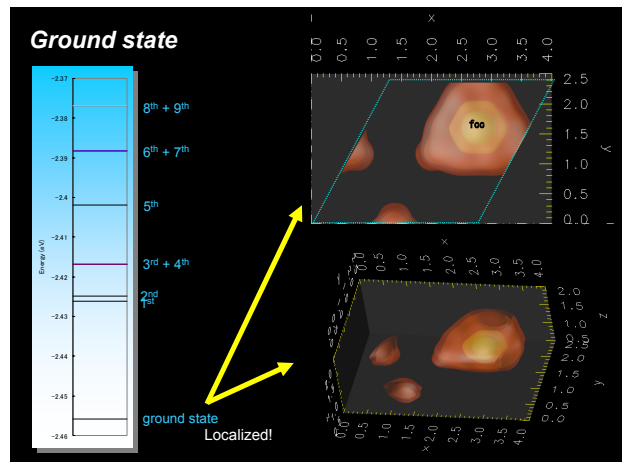
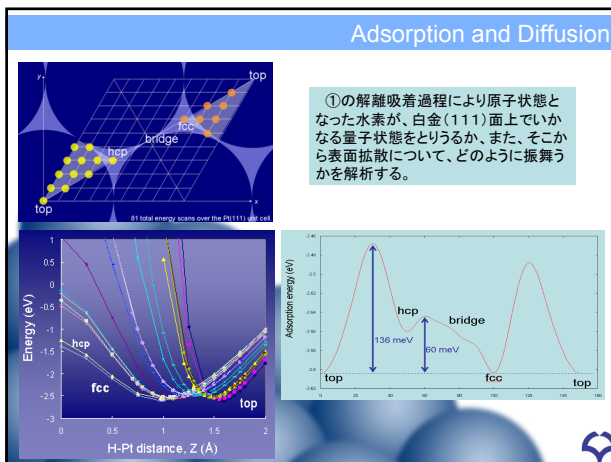
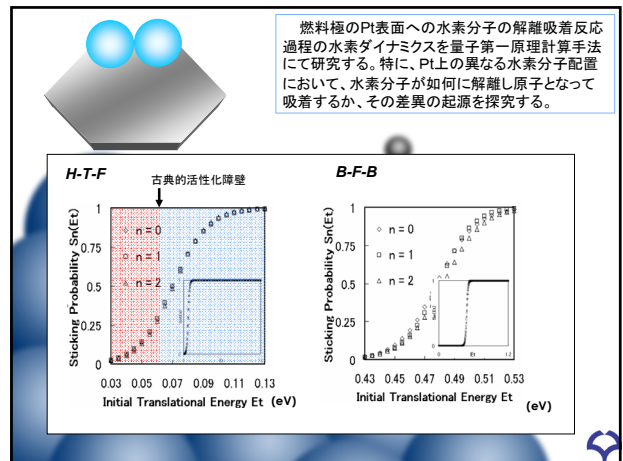
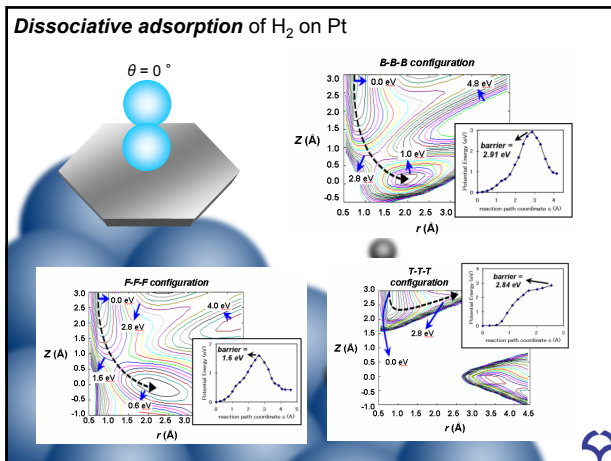
Dissociative adsorption of H₂ on Pt

$\theta = 90^\circ$

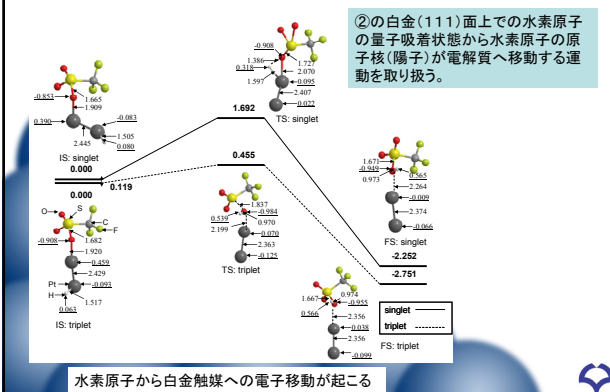


H-B-F configuration

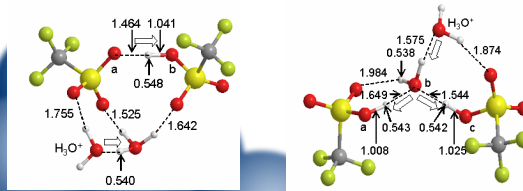
H-T-F configuration



③ Dynamics of proton liberation from the Pt surface



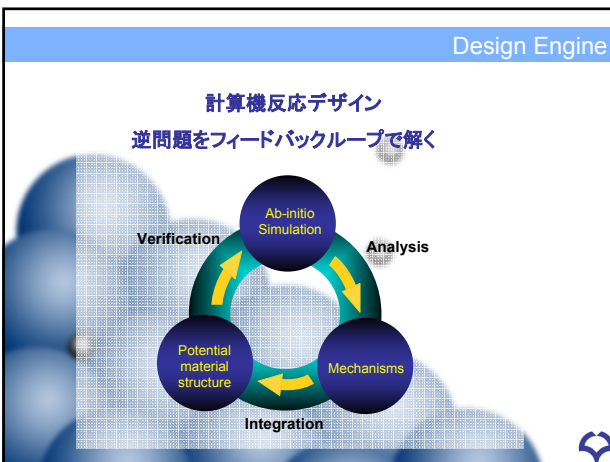
Proton conduction in the Proton Exchange Membrane (PEM)



側鎖間の直接的な伝導

側鎖間の間接的な伝導

H₂O分子を介し、O-H結合の内部変換を伴う



Cyclic hydrocarbon dehydrogenation catalyst design

