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# 第一原理分子動力学法による電極界面のシミュレーション

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## STATE-Senri

## (Simulation Tool for Atom TEchnology)

- Density Functional Theory
  LDA、GGA、LDA+U
- Ultrasoft pseudopotential
- Plane wave basis set
- Iterative diagonalization
  Davidson法、RMM-DIIS法
- Broyden charge density mixing

→ Applied to wide range of materials

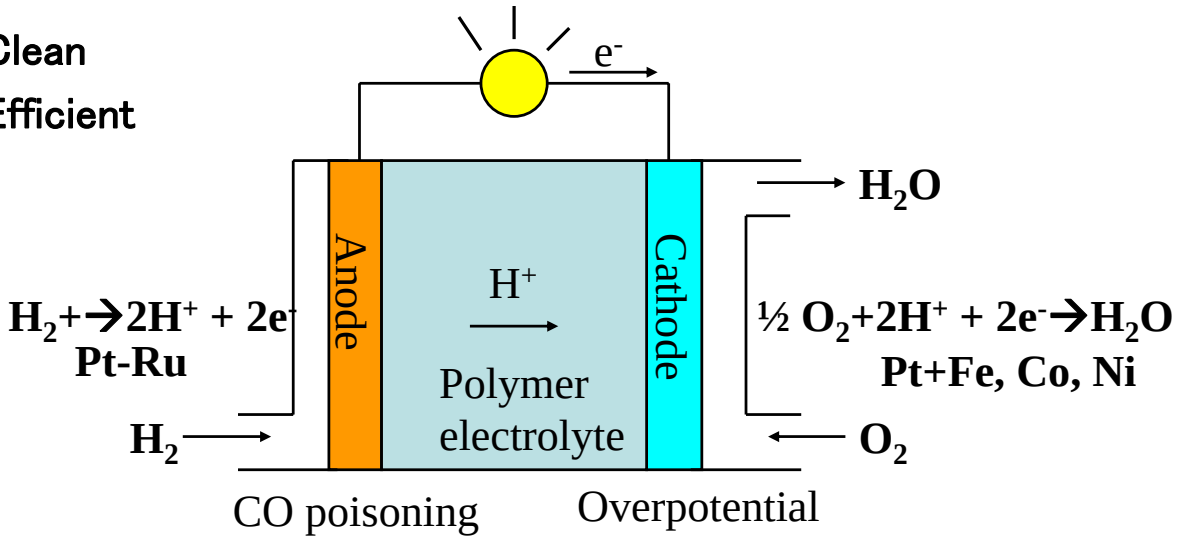
- **Tutorial course in "Computational Materials Design (CMD) Workshop".**
  http://www.dyn.ap.eng.osaka-u.ac.jp/CMD110/
- Twice a year
  Sep. 11th–15th, 2007 and Mar. 4th–8th, 2008
- Open to both theoretical and experimental researchers.
- Open to Asian researchers and students.

# Fuel Cell

**Polymer Electrolyte Fuel Cells.**

**Clean**

**Efficient**




Electrode metals

- Pt: South Africa74%、Russia14%

→New efficient catalysts are required.

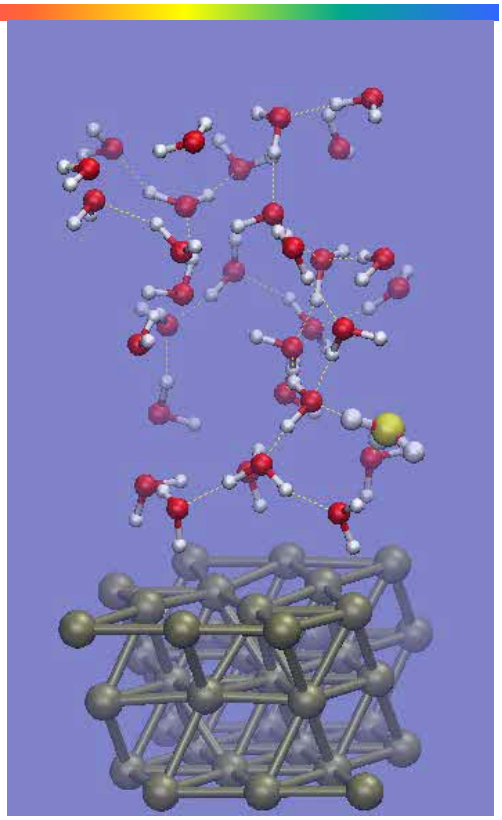
→Necessary to elucidate the reaction mechanisms.





# MD simulation of electrode/water interface

- Total MD simulation time: 3.2 ps
- Added electrons: 0.25–0.40
- 353 K

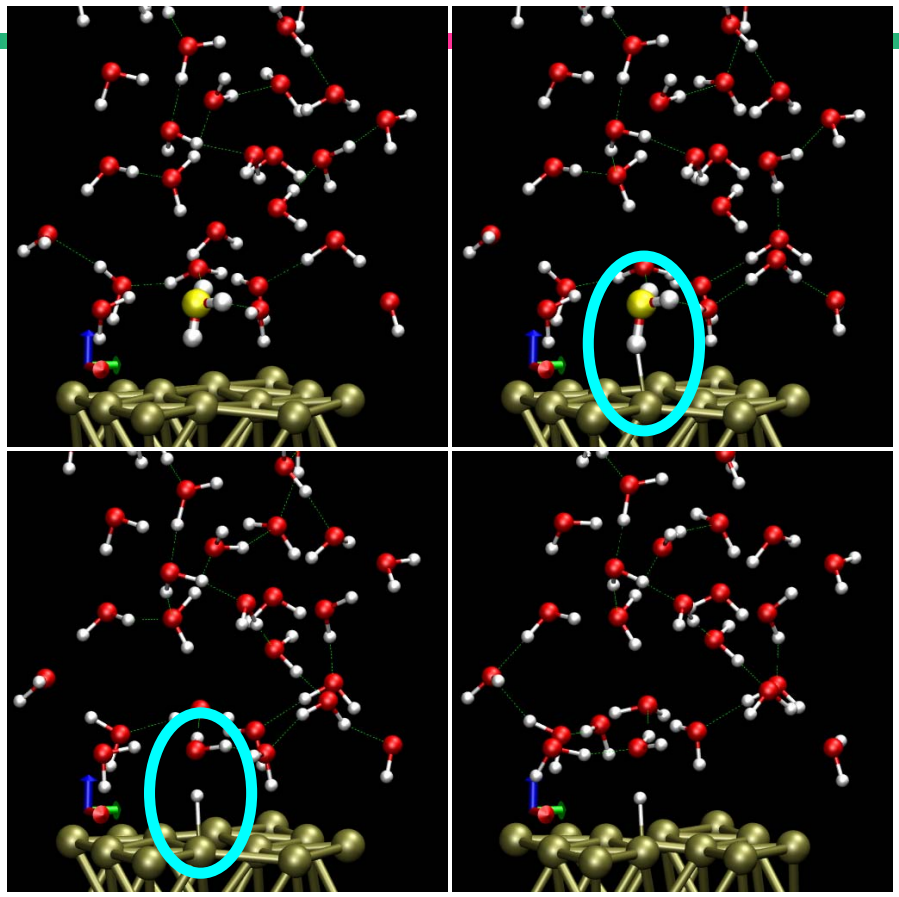


Red: Oxygen

White: Hydrogen

Yellow: Oxygen in a hydronium ion

Substrate: Platinum





# Organic based devices

- Important in applications of organic based devices such as organic light-emitting diodes (OLED), organic photovoltaic cells, organic field effect transistors, and so on.
- The performance and efficiency of those organic-based devices critically depend on the electronic structures at organic/metal interfaces.



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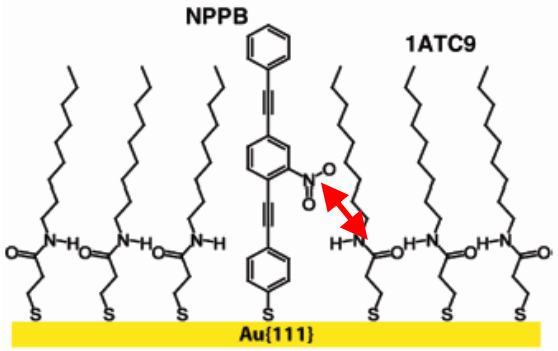
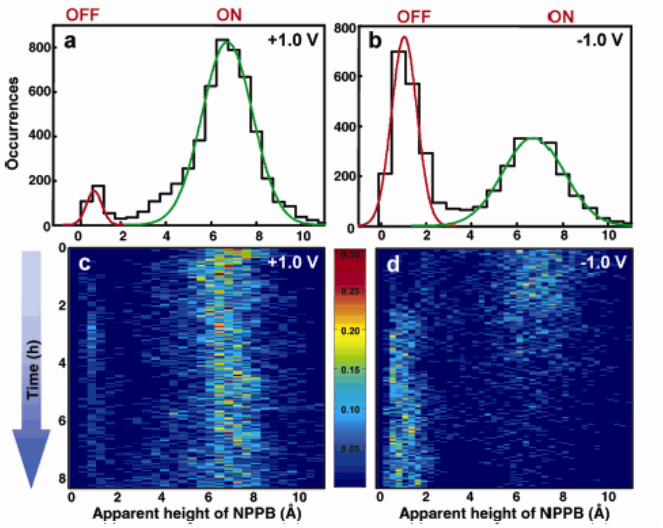
# Molecular Switch




- 4-(2'-nitro-4'-phenylethynyl-phenylethynyl)-benzenthiol (NPBB)
  P.A.Lewis *et al*, JACS 126 12214 (2004), *ibid* 127, 17421 (2005).
- Positive Sample Bias → ON
- Negative Sample Bias → OFF

**Electric Field**
**Hydrogen bond.**



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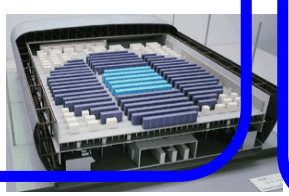
EARTH SIMULATOR



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