# Functional Nano-particle Simulation


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*Nano-particle* which means a fine particle in nanometer scale is promising material for several industrial applications. *Nano-particle* consisting of transition metals seems to be a good catalyst used in DMFC (direct methanol fuel cell). Conventional catalyst for decomposition of methanol is made of platinum, and, recently, platinum-based alloys containing transition metals are introduced. However, there are confusing arguments concerning a role of the transition metals. In order to develop a new stable and highly efficient catalyst in the DMFC, it is an urgent problem to explain the role in the catalysis reaction. We investigated electronic structures of Ru(0001) surface and CO molecule absorbed on the Ru(0001) surface. The electronic structure calculation was carried out based on the density functional theory with the PBE96 formula for the exchange-correlation energy functional. The atomic positions were determined quantum mechanically, i.e. the first-principles molecular dynamics method was used. Actual performance of the present code, PHASE Ver.5.0, shows 0.9TFLOPS using 32 nodes of the Earth Simulator. Before we describe the results of CO absorption on Ru surface, let us summarize the simulation results of $O_2$ dissociation process on the Ru(0001) surface. In the present case, the $O_2$ molecule is dissociated without any energy barrier. On the other hand, the $O_2$ molecule does not dissociate and absorbs as a molecule on Pt surface. We experimentally confirmed these facts by using the SPring-8. As for the Ru(0001) surface with a partial oxidation, we investigated the CO absorption process, where one Ru atom is substituted with other transition metal atom, Zr, Nb, Mo, Tc, Rh or Pd. The calculated absorption energy of the CO molecule on the surface depended on the kind of the substituted atom, and showed a clear chemical trend. It is expected that these numerical results give a clue to synthesize a new catalyst in industrial development phase.



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