# Modeling of $TiO_2$ nanoparticles interactions with water and ions

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Although $TiO_2$ is not a major rock-forming mineral, it is an important technological material, and it has been used extensively as a model for oxide-water studies. Because the surfaces of the common $TiO_2$ phases, rutile and anatase, have been characterized experimentally and modeled with density functional theory (DFT), they serve as good model systems for understanding the size and shape effects of nanoparticles on the oxide-water interface.

In this talk, we will present results of DFT calculations on rutile and anatase surfaces and nanoparticles interactions with $H_2O$. The relationship of surface site defects (i.e., corner and edge sites) to $H_2O$ adsorption energy is investigated. DFT calculations on anatase surfaces with adsorbed ions are also presented.

These DFT calculations were then used in developing a reactive classical force field, ReaxFF, for the Ti-O-H system. The ReaxFF was used to perform molecular dynamics simulations of rutile and anatase particles in water and aqueous salt solutions. Differences in the electrical double layer around finite nanoparticles as compared with flat, infinite surfaces will be discussed.

# Hybrid Pressure Coring System of D/V *Chikyu*

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Pressure coring is a technique to keep *in-situ* conditions in recovering subseafloor sediment samples, which are potentially rich in soluble or hydrated gas. Gas fractions are easily lost in regular core sampling through the pressure and temperature change during core recovery, and subsequently change the chemical components of the sample: e.g., degassing may cause critical changes and/or damages of original structures. To study original characteristics of gaseous subseafloor sediment, a New Hybrid Pressure Coring System (Hybrid PCS) was developed for the D/V *Chikyu* operation by adapting some of the existing pressure sampling technologies. Hybrid PCS is composed of three main parts: top section for the wireline tool, middle section for the accumulator and pressure controlling system, and the bottom section for the autoclave chamber. The design concept is based on that of Pressure Core Sampler used in Ocean Drilling Program, and of Pressure Temperature Core Sampler (PTCS) and Non-cooled PTCS of Japan Oil, Gas and Metals National Coporation (JOGMEC). Modifications were made on the ball valve, which operates to close the autoclave after coring. The core samples are 51 mm in diameter and up to 3.5 m in length. The system is combined with the Extented Shoe Coring System on the *Chikyu* and best suited for coring of semi-consolidated formation up to about 3400 m from the sea level. Sample autoclave is compatible with Pressure Core Analysis and Transfer System of Geotek Ltd for sub-sampling and analysis under *in-situ* pressure. The analysis includes X-ray CT scan and core logging with P-wave velocity and gamma density. Depressurization provides accurate volume of gas and its sub-sampling.

Hybrid PCS was first tested during the *Chikyu* Exp. 906 at a submarine mud-volcano in the Nankai Trough. A 0.9 m of hydrate rich material was recovered from the summit (water depth: 2000 m) and the intact hydrate structure was observed by X-ray CT scan. Hybrid PCS was also used in the following JOGMEC methane hydrate cruise, resulting in the good recovery of methane hydrate-bearing cores (approx. 69%).

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