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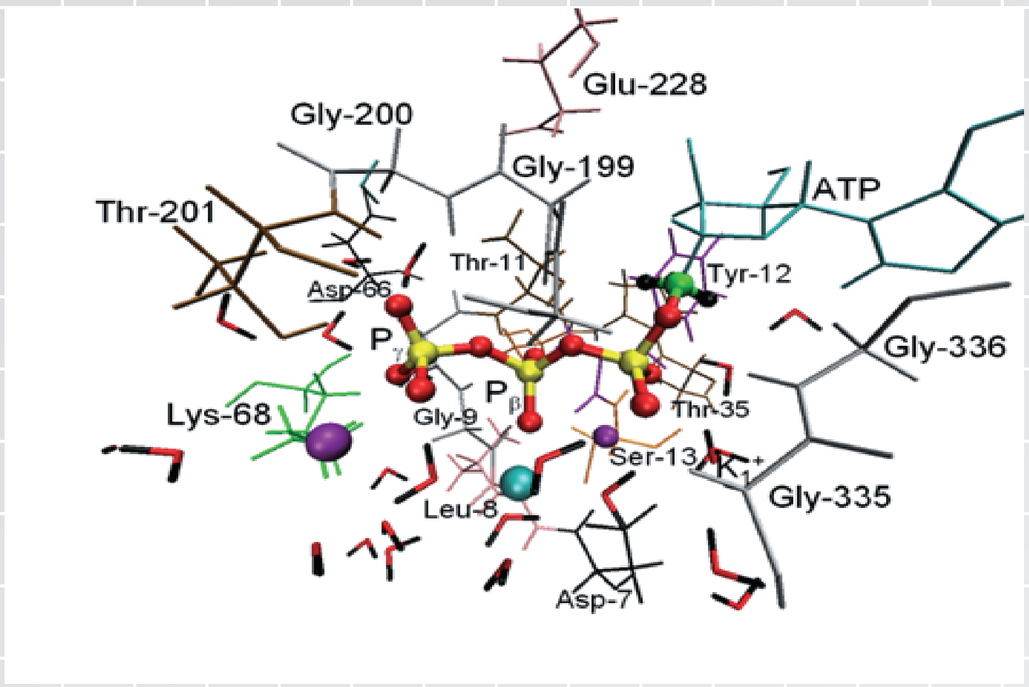
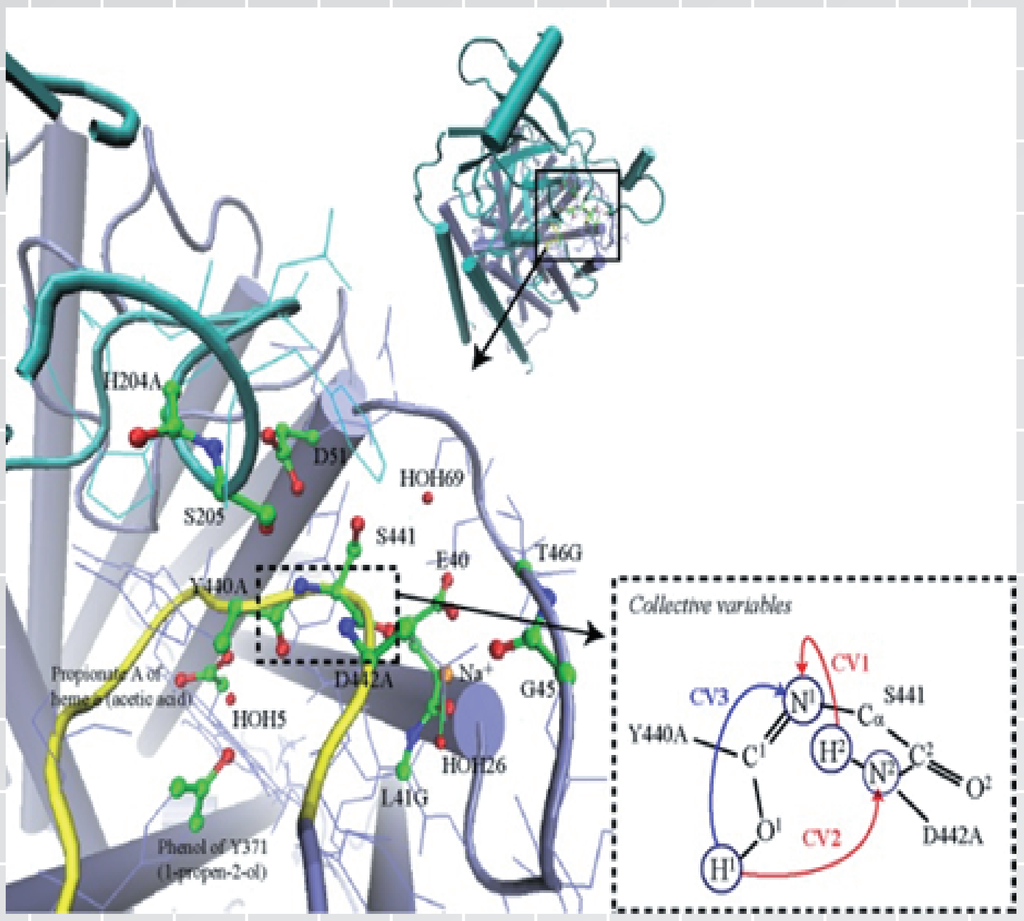
Computational Materials and Life Sciences

ATPase in Hsc70 protein

QM/M simulations, coupled to metadynamics, on Hsc70 ATPase protein, show how a water molecule coordinated to Mg^{2+} acts as a catalyst and evidence the unique and cooperative role of K^+ and Mg^{2+} metal ions in promoting the release of the inorganic phosphate via an exchange of OH^- between their respective solvation shells.





Cytochrome *c* Oxidase

The mechanism of a proton transfer across a peptide group in bovine cytochrome *c* oxidase has been investigated via metadynamics. The results provide support to a recently proposed H-path in the general cell respiration process and show how a double H^+ transfer between two adjacent peptide groups results in a modest activation barrier and is consistent with the X-ray data.

Computational Approach to Nano Materials

Magnetic Carbon Nanotubes

Experimental observations of magnetism in nanometer carbon materials have stimulated a lot of attentions to carbon allotropes as promising candidates for light and stiff magnetic materials which are expected to be applicable to a wide field of modern technology. Vacancies, edges, and negative Gaussian curvature introduced in the honeycomb networks of sp^2 C atoms have been known to result in the magnetism on sp^2 carbon nano-materials.

Here we design a new magnetic carbon nanotube with topological line defect consisting of pentagon and octagon rings by performing the first-principles total-energy electronic-structure calculations in the density functional theory (DFT). Our DFT calculation certainly show that the nanotube with the topological line defect exhibits magnetic ordering that polarized electron spins are localized around the defect and ferromagnetically aligned along the tube axis. The calculated magnetic moment is about 0.04 μ_B/Å irrespective of the tube diameter studied here.