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Charge transfers from Na atom in (H2O)n clusters and in water solution TAKESHI NOZUE, JUNICHI HOSHINO, KAZUO TSUMURAYA, Meiji University — The charge state of sodium ions in water is an essential issue in both biophysical and physicochemical areas. Although the nominal charge state of sodium is +1 in water solution, the true charge is less than unity and will depend on the environments. We clarify the true charges states with ab initio density functional methods. There have been several methods to evaluate the charges that belong to each atom in molecules: Bader analysis divides up into regions where the dividing surfaces are at a minimum in the density. [1] The Bader charge analysis [2] has difficulty of finding all the critical points around the atom. Henkelman et al. have proposed a modified partition scheme. [3] We use a modified version of the Henkelman's scheme to integrate the core charge densities separately. The method gives the charge transfer from Na to H2O to be 0.167e and that to (H2O)2 to be 0.522e. The original Bader charge scheme gives 0.156e and 0.596e respectively. We present the transfers surrounded by a large number of water molecules and those in water solution in periodic system. [1]R.F.W.Bader, Atoms in Molecules: A Quantum Theory, Clarendon:Oxford. 1990. [2]C.F.Guerra, et al., J.Comp.Chem. 25, 189(2003). [3]G.Henkelman, et al., Comp. Mat. Sci. in press.

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