

Research keywords: Crystallography, intermolecular interactions, hydrogen bonds, crystal design.

We are interested in the intermolecular interactions involving polyoxometalates. Main topics include (i) solid-state and solution structures of hydrogen-bond assisted polyoxometalate aggregates, (ii) crystal design of nano-scale polyoxometalates, and (iii) design of molecular composites consisting of polyoxometalates and silver ethynide clusters.

(i) Hydrogen-bond assisted polyoxometalate aggregates: We showed that protonated decavanadates,  $H_n V_{10} O_{28}^{(6-n)-}$ , exhibit cation- and solvent-dependent various hydrogen-bonding aggregates in crystals [1] and such aggregates are transferred into the solution phase [2]. Multinuclear NMR and small angle X-ray scattering (SAXS) demonstrated that hydrogen-bonded oligomer formations are reversible and depends on the nature of the solvents.

(ii) Crystal design of nano-scale polyoxometalates: Controlled crystallization of wheel-type and spherical nano-scale polyoxometalates allowed us to reveal their nuclearity growth and crystallization mechanisms [3] and to construct crystals with huge water channel with the diameter of 3 nm [4]. Analyses of these structures were made possible by the synchrotron X-ray diffraction.

(iii) Design of molecular composites: We are extending our study to the intermolecular interactions of polyoxometalates with other kinds of cluster compounds. With the combination of silver ethynide clusters, we have demonstrated that the molecular composites can rationally designed by controlling the structures of the polyoxometalates [5, 6].

## Possible collaborations

We can offer our state-of-the art synchrotron single-crystal X-ray diffraction experiences. Also, any collaborations using our compounds are welcome.

References. [1] Nakamura & Ozeki, J. Chem. Soc., Dalton Trans., 2001, 472. [2] Kojima, Antonio & Ozeki, J. Am. Chem. Soc., 2011, 133, 7248. [3] Shishido & Ozeki, J. Am. Chem. Soc., 2008, 130, 10588. [4] Saito & Ozeki, Dalton Trans., 2012, 41, 9846. [5] Kurasawa, Arisaka & Ozeki, Inorg. Chem., 2015, 54, 1650. [6] Tamari, Ono, Hashimoto & Ozeki, Dalton Trans. 2015, 44, 19056.