

## **Presentations**

- [1] M. Takano (invited), Coulombic viewpoint of how molecular motors work, Biophysical Society of Japan 53th Annual Meeting, Kanazawa, Sept. 14, 2015.
- [2] J. Ohnuki, T. Sato, and M. Takano, Electrostatic and allosteric response of myosin as a mechanosensor, Biophysical Society 60th Annual Meeting, Los Angeles, Feb. 28, 2016.
- [3] T. Sato, J. Ohnuki, and M. Takano, Electrostatic and allosteric response of myosin upon ATP binding, Biophysical Society 60th Annual Meeting, Los Angeles, Mar. 1, 2016.
- [4] D. Parkin, Y. Mizuhara, and M. Takano, Salt bridge stability in the generalized Born model, Biophysical Society of Japan 53th Annual Meeting, Kanazawa, Sept. 14, 2015.

## **Research Summary**

- By MD simulation and the numerical calculation of the Poisson equation, we elucidated the role of the Coulombic interaction in the force generating function of molecular motors.
- By using the replica exchange umbrella sampling method, we found piezoelectricity in myosin, a well-known molecular motor, and showed that the piezoelectricity is likely to contribute to the force generation and its regulation at the nanometer scale.
- By MD We found that myosin exhibits significant dielectric response, which is also likely to contribute to the force generation and its regulation.
- We clarified how the integration range for the electrostatic energy density in the generalized Born model affects the electrostatic interaction between opposite charges.