Presentations

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.