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Computational Study of Force-Gating in Myosin VI IAN LOWE, YUBO YANG, RIINA TEHVER, Denison University — Myosin VI is a molecular motor whose processivity is achieved via mechanical gating of its ATPase activity. The goal of our work is to elucidate the gating mechanism at molecular level. We have performed Brownian dynamics simulations to probe this mechano-chemical coupling within the motor domain. To reach biologically relevant timescales, we use coarse-grained models for myosin VI, both with and without explicit ATP. Our model also allows us to explicitly include external mechanical stress and study the response of the motor and its ATP binding pocket while tuning the external force parameters.

Riina Tehver
Denison University

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