

(a)

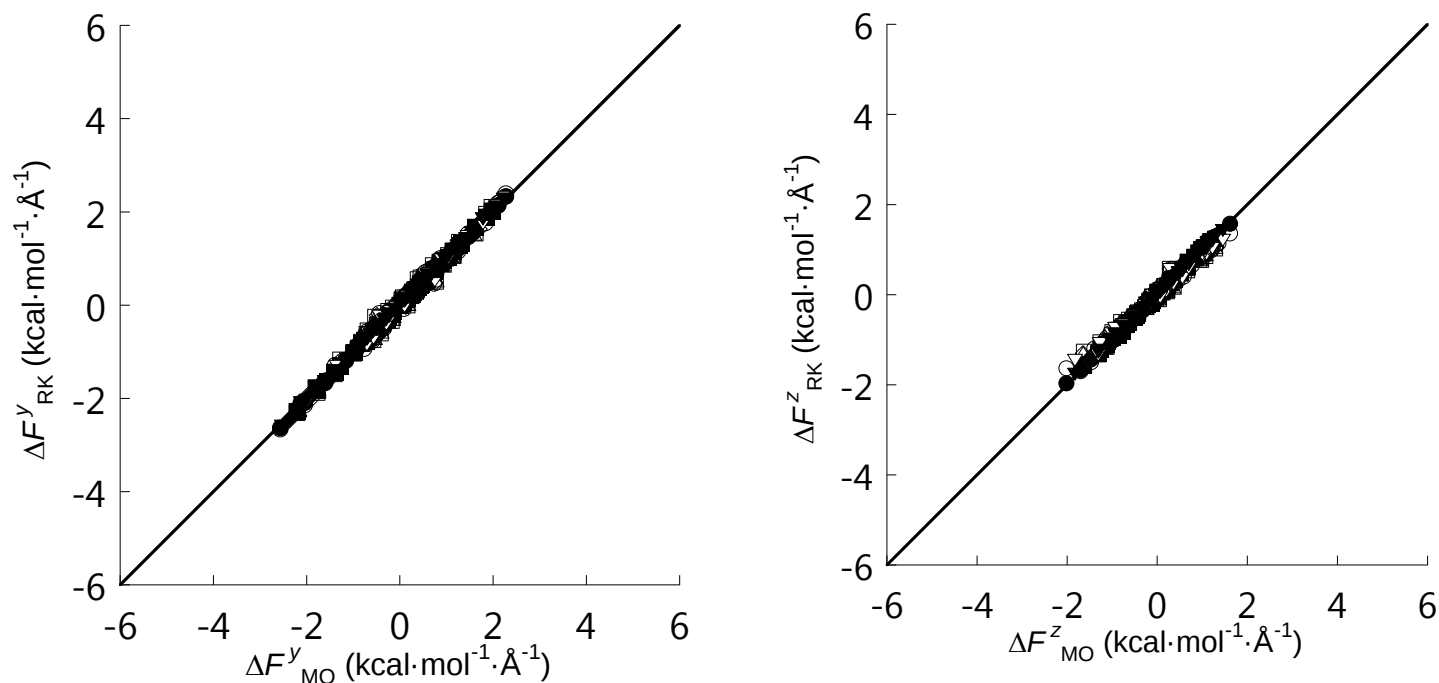


Fig. S1.

Comparison of induced forces to the y and z directions, ΔF^y and ΔF^z , between response kernel (RK) and MO calculations for different wave functions. Opened and filled symbols mean CRK and CDRK results, respectively, for water molecule. (a) induced forces on QM atoms, and (b) induced forces on test charges are depicted. HF($\bigcirc$), MP2($\diamond$), CCSD($\square$), B3LYP($\triangle$), and M06(∇). Basis sets used are 6-311G(2d,2p).

(b)

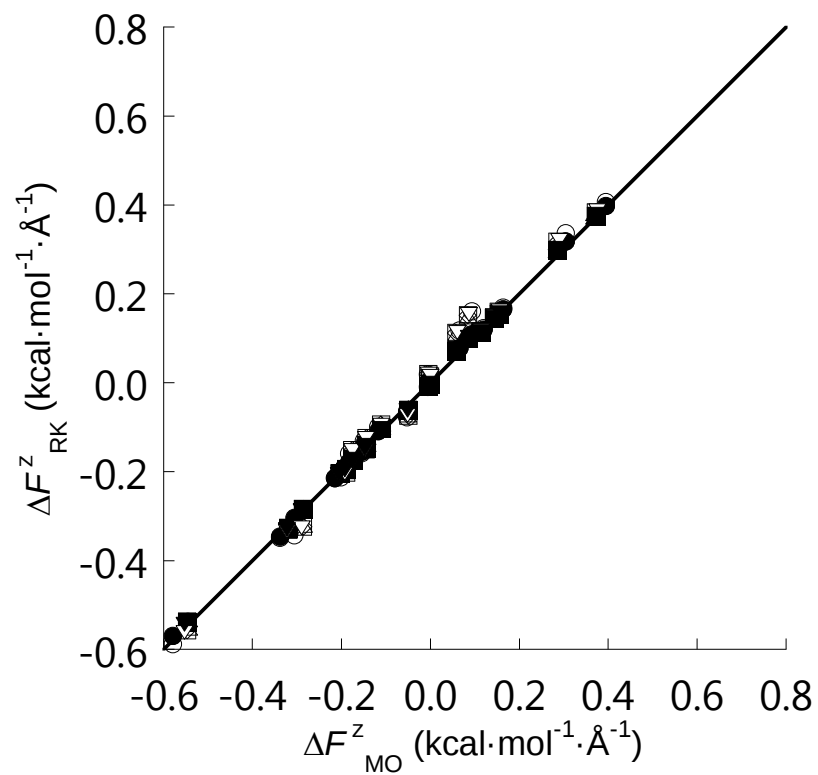
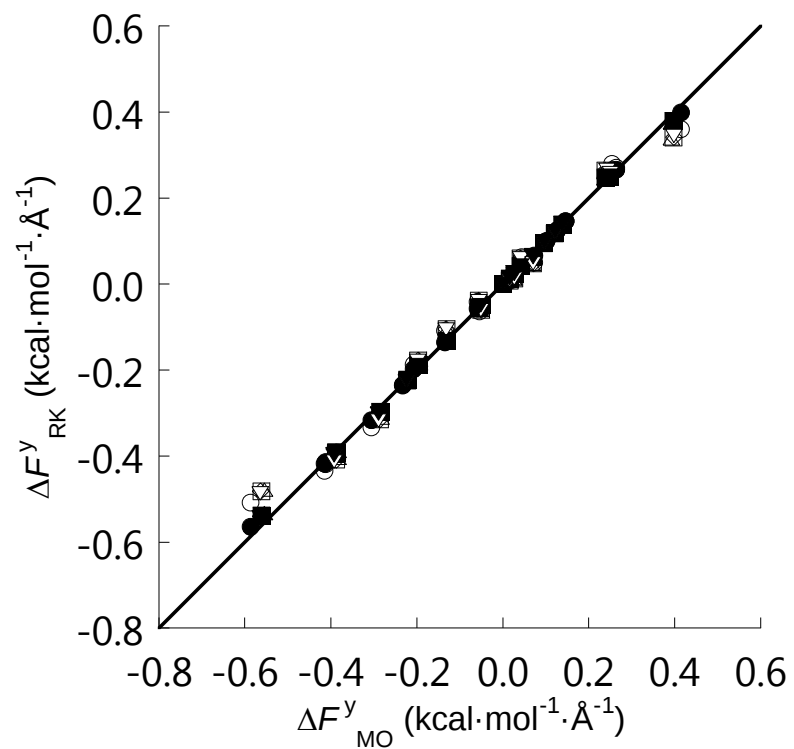


Fig. S1.
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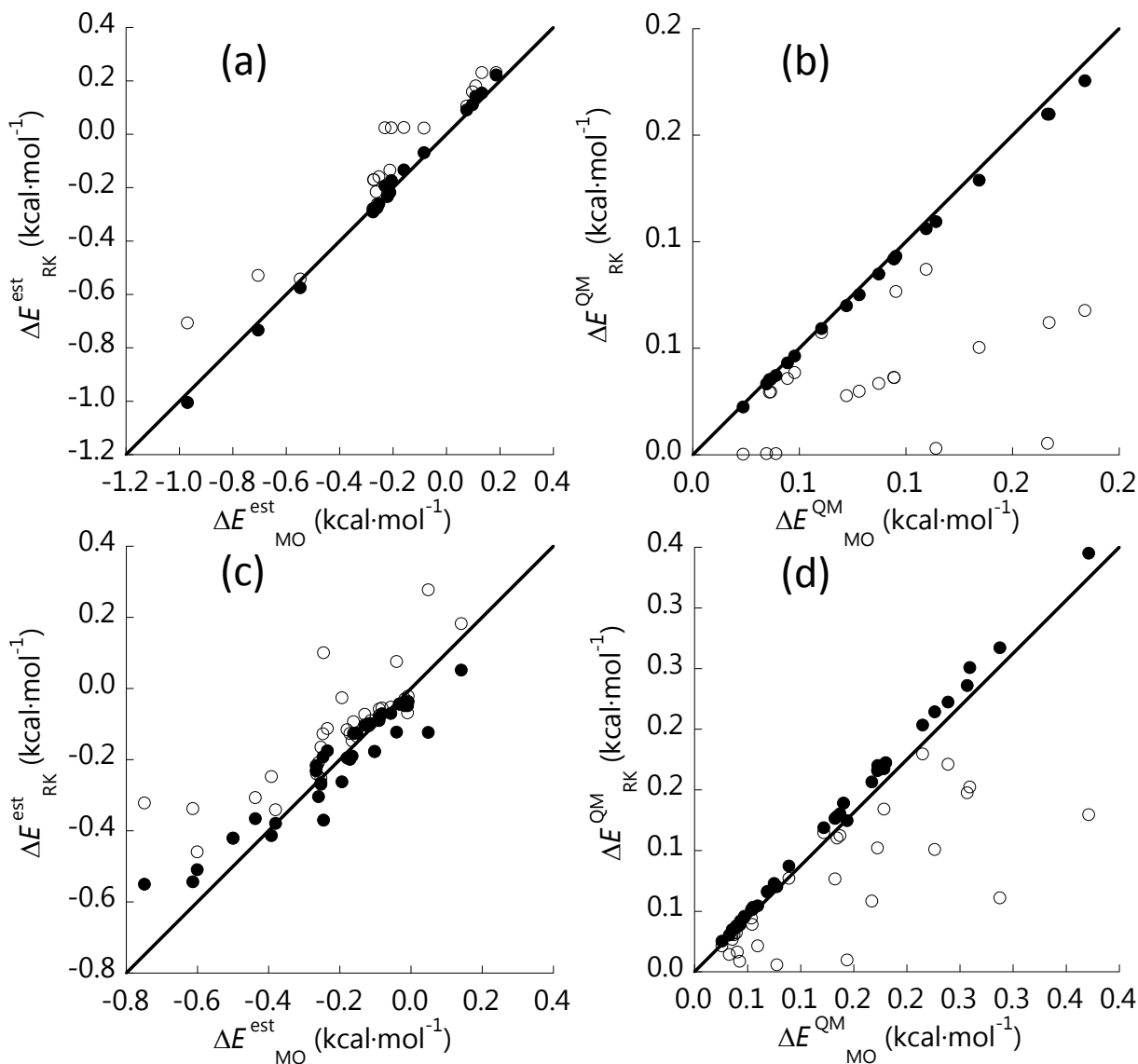


Fig. S2.

Comparison of induced electrostatic (ΔE^{est}) and internal (ΔE^{QM}) energies between response kernel (RK) and MO calculations for MP2/aug-cc-pVDZ. Opened and filled circles mean CRK and CDRK results, respectively. (a) ΔE^{est} of CO_2 , (b) ΔE^{QM} of CO_2 , (c) ΔE^{est} of ethylene, (d) ΔE^{QM} of ethylene.

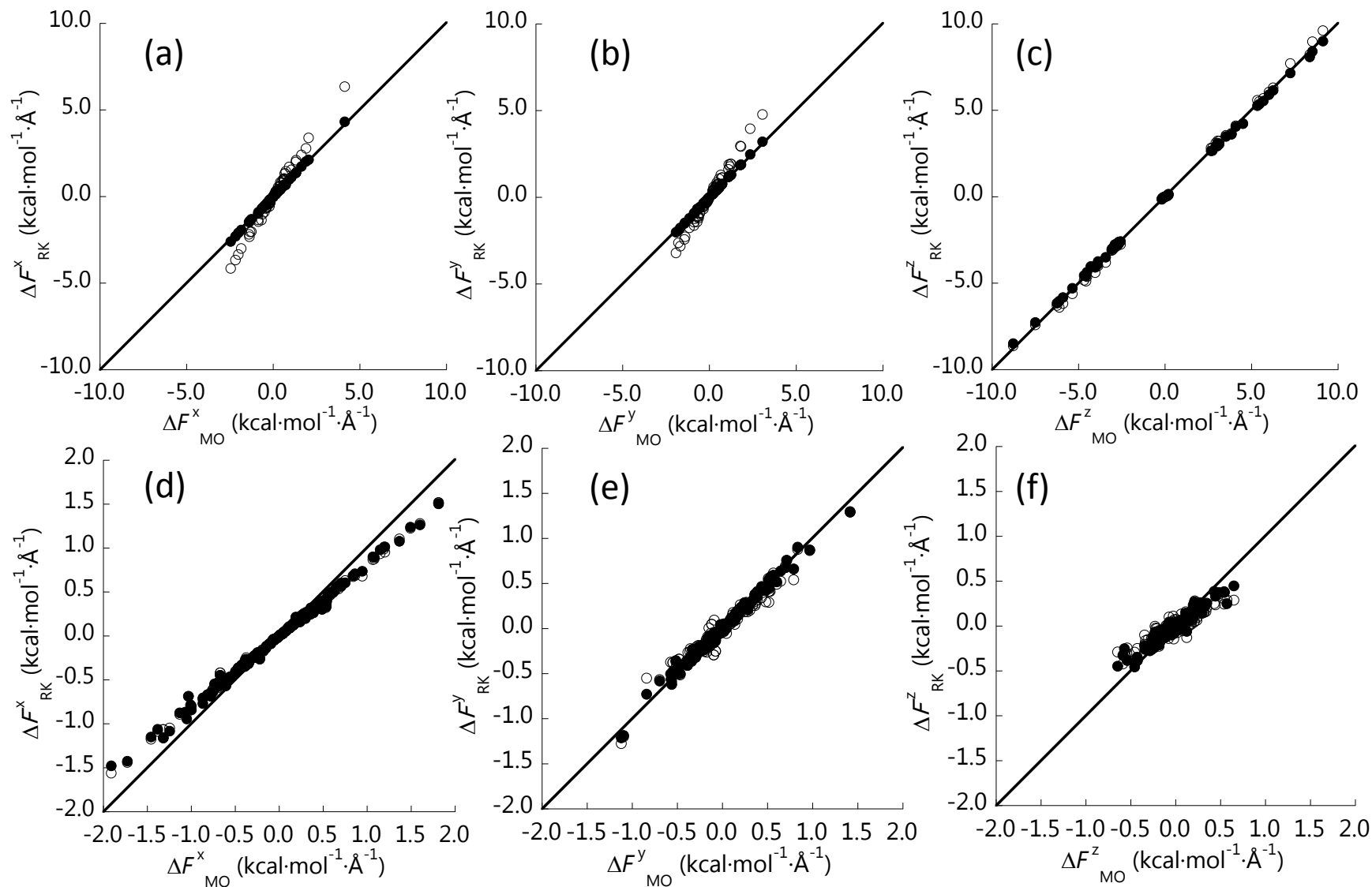


Fig. S3.

Comparison of induced forces $\Delta F^{\{x,y,z\}}$ along each axis between response kernels (RK) and MO calculations for MP2/aug-cc-pVDZ. Opened and filled circles mean CRK and CDRK results, respectively. (a) ΔF^x of CO_2 , (b) ΔF^y of CO_2 , (c) ΔF^z of CO_2 , (d) ΔF^x of ethylene, (e) ΔF^y ethylene, (f) ΔF^z of ethylene. Z axis is bond direction and principle axis in CO_2 and benzene, respectively.

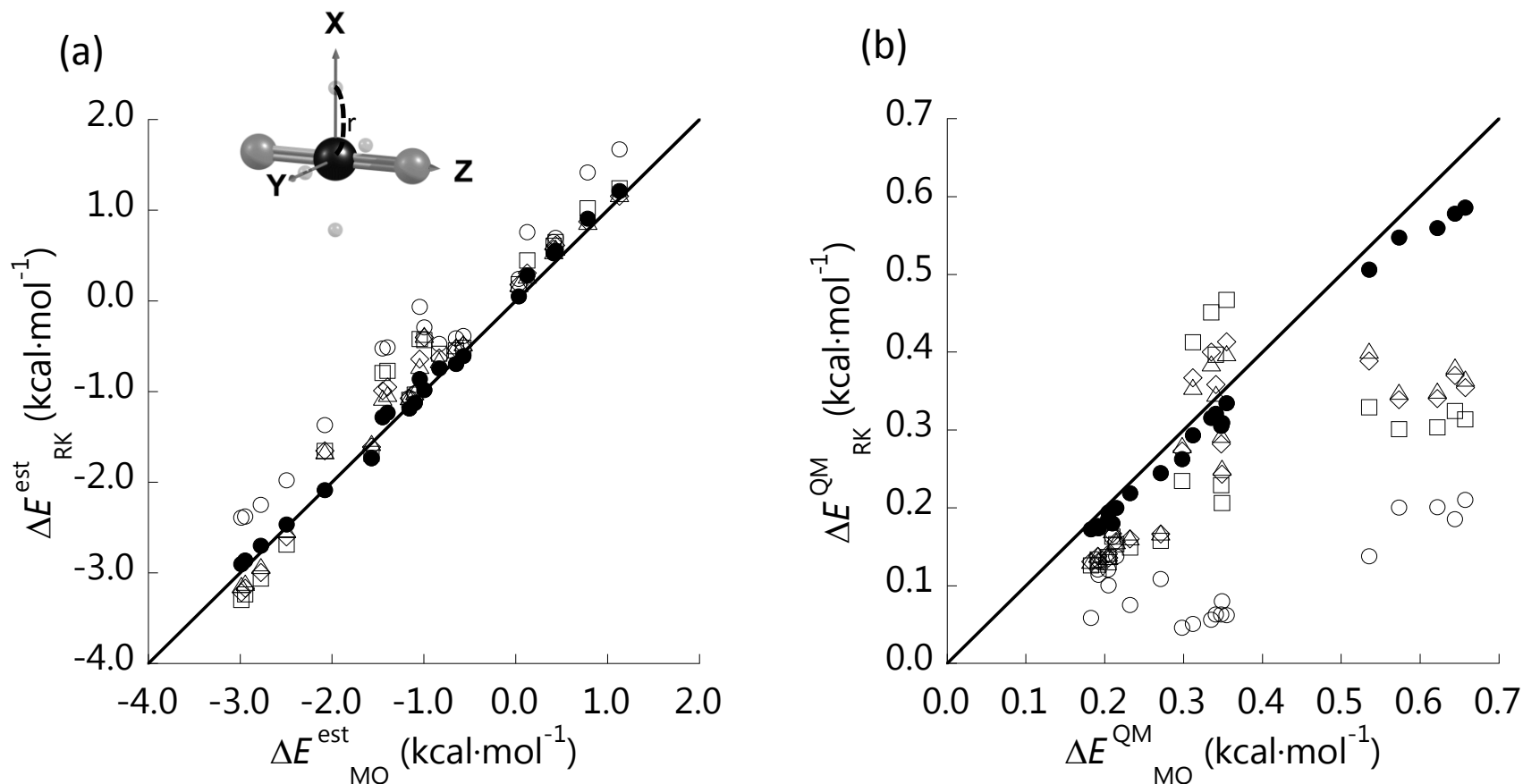


Fig. S4.

Comparison of induced electrostatic (ΔE^{est}) and internal (ΔE^{QM}) energies between response kernels (RK) and MO calculations for MP2/aug-cc-pVDZ. Opened and filled symbols mean results of CRK with imaginary sites and results of CDRK model, respectively. In the CRK model, four imaginary sites are placed at the position perpendicular to the bond 0.2(Δ), 0.5($\diamond$), 1.0($\square$) angstrom far from the carbon atom. Open circle means the basic CRK model with no imaginary site. (a) ΔE^{est} of CO₂, (b) ΔE^{QM} of CO₂ are depicted.

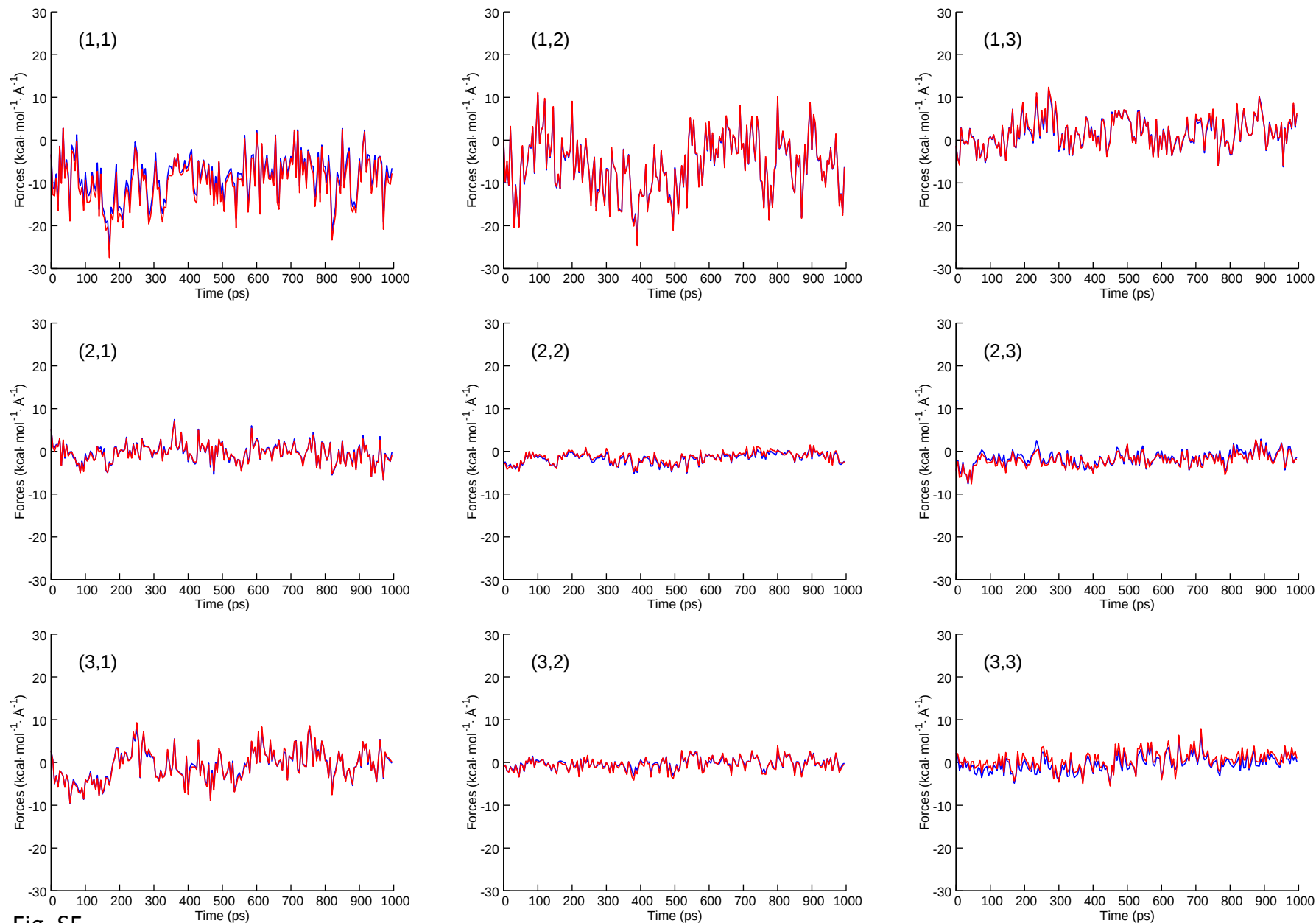


Fig. S5. Comparison of forces on QM atoms (see Fig. 7) between CDRK (red) and QM (blue) methods for different MM configurations obtained by MM MD simulation using CDRK model prepared by M06-2x/6-311G(d). The figure index (m,n) means that F_x ($n=1$), F_y ($n=2$), and F_z ($n=3$) components of forces on m-th QM atoms.

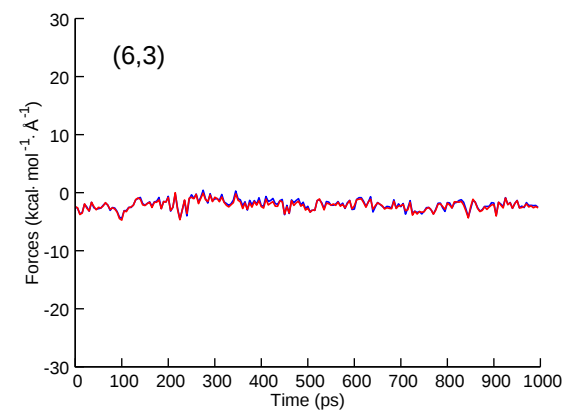
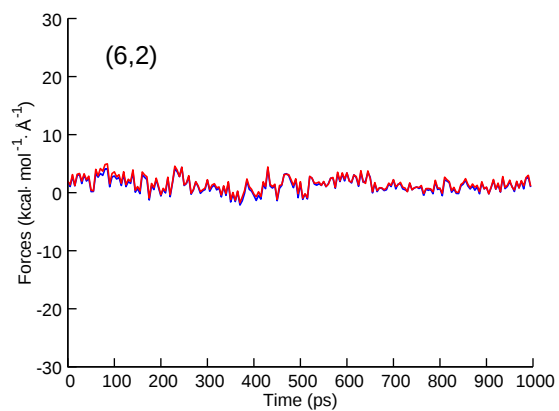
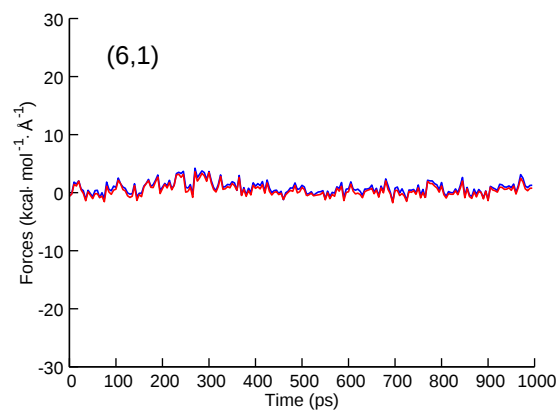
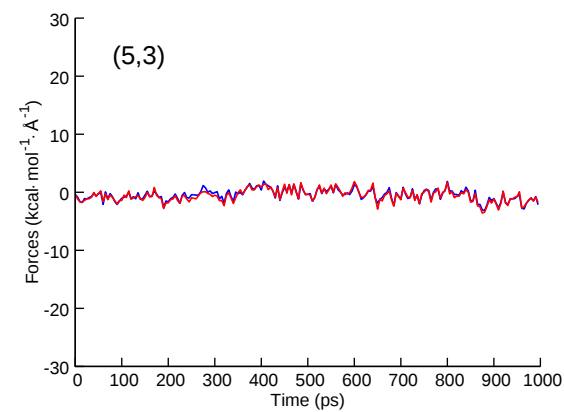
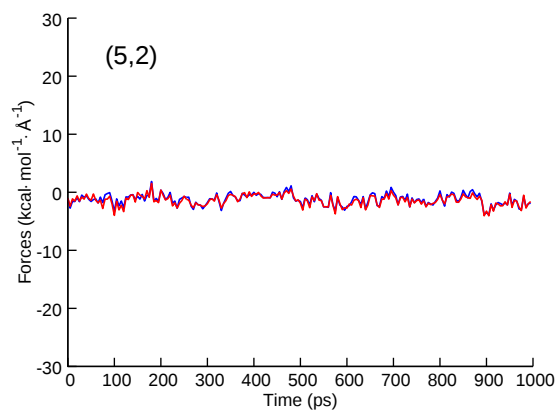
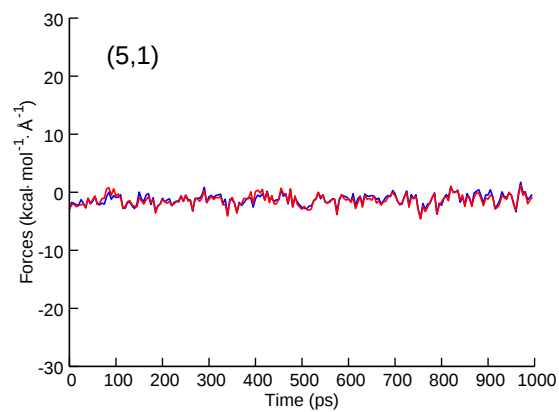
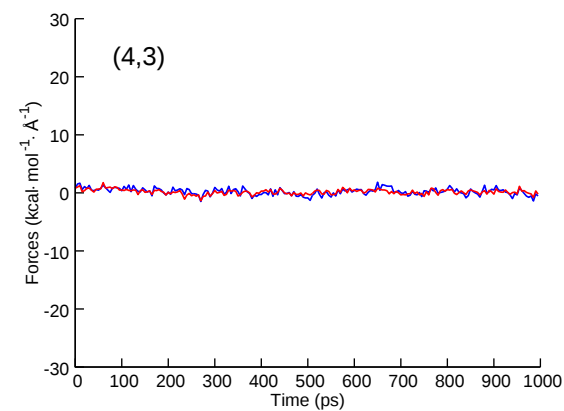
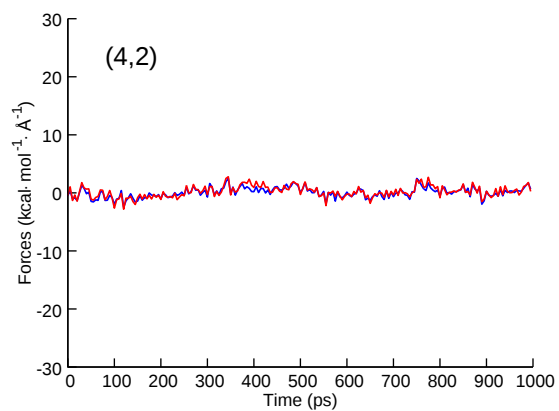
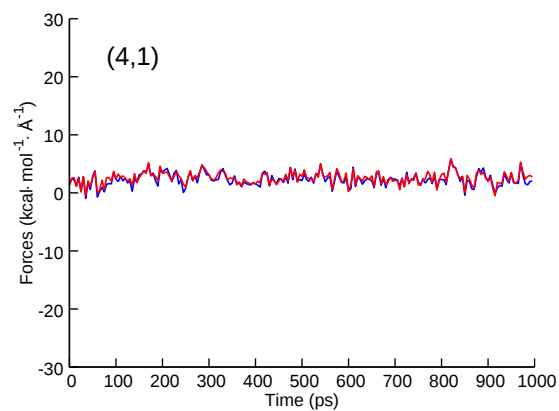


Fig. S4.
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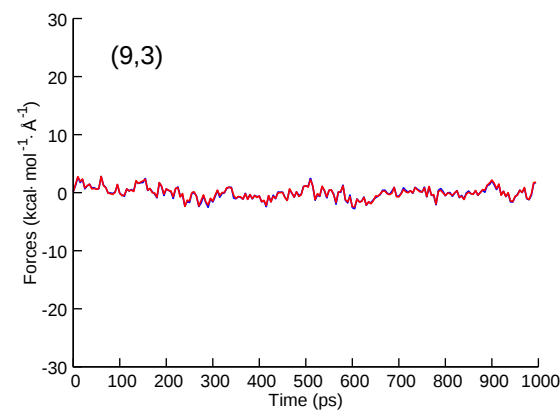
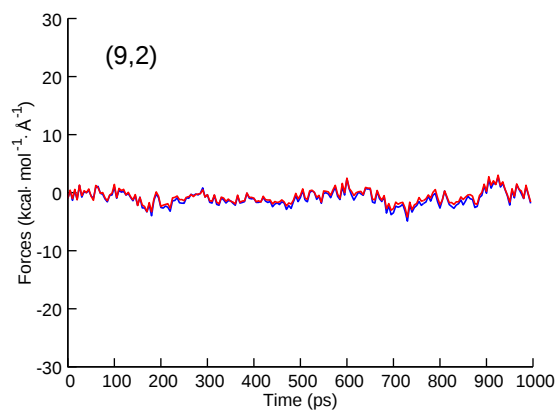
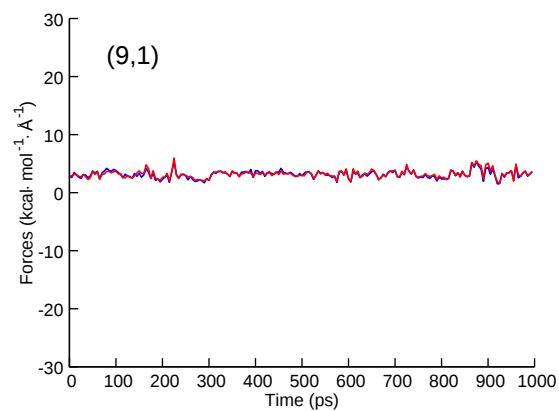
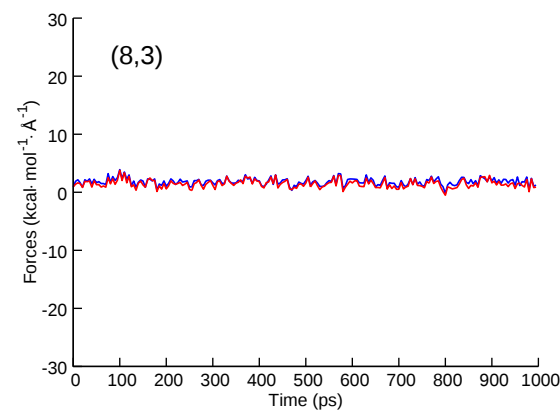
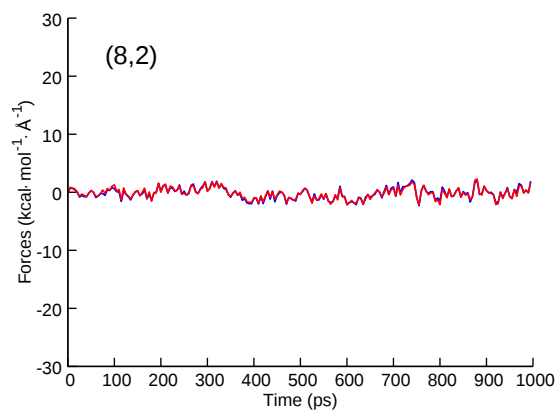
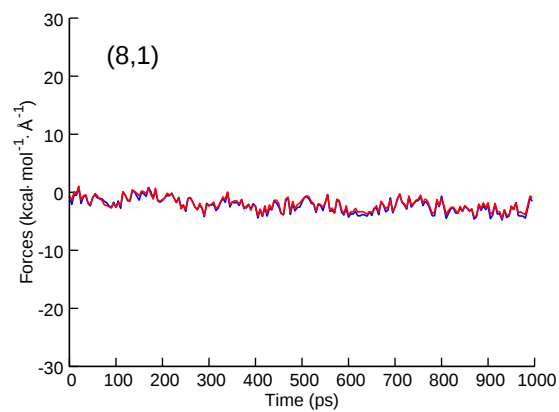
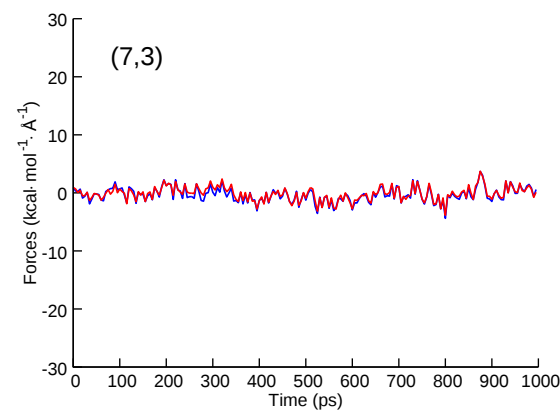
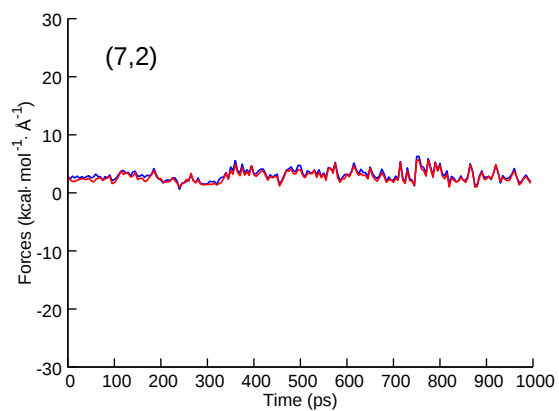
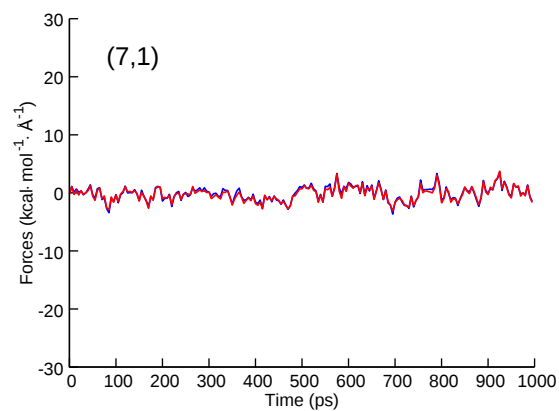


Fig. S4.
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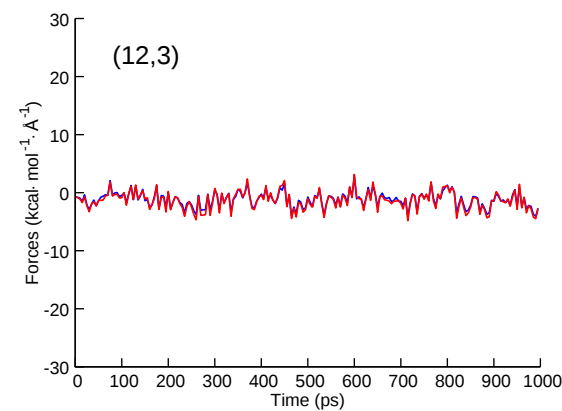
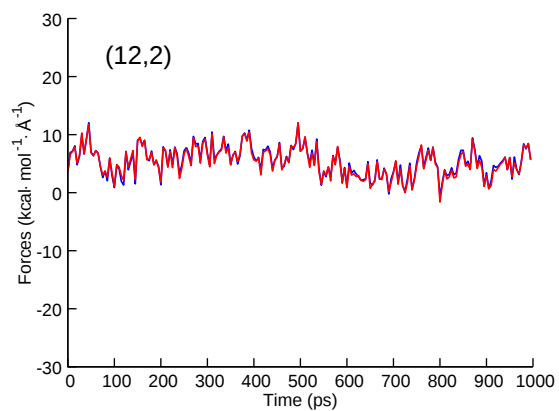
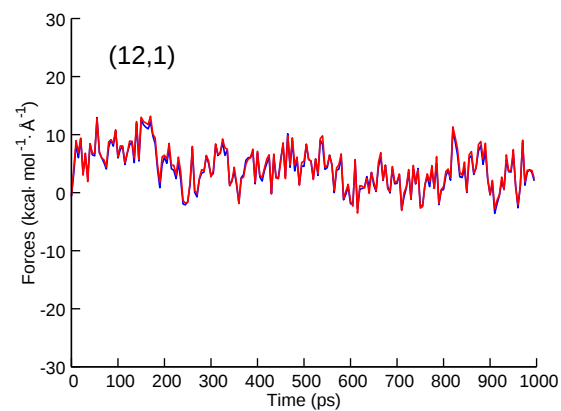
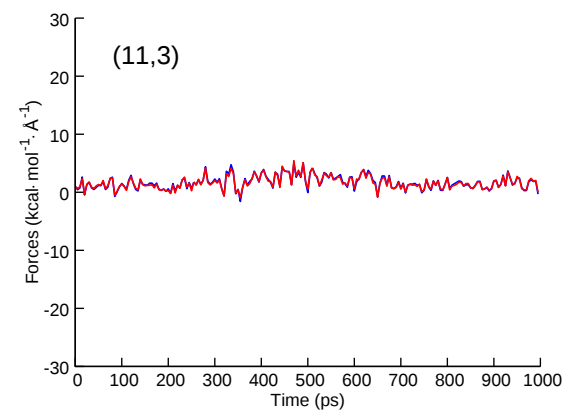
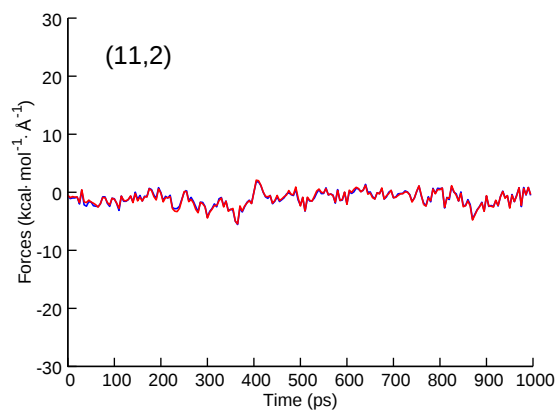
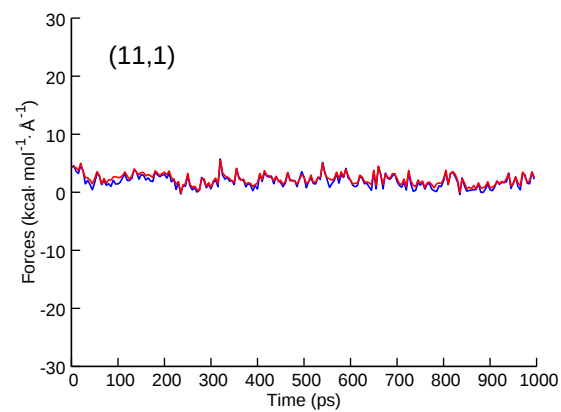
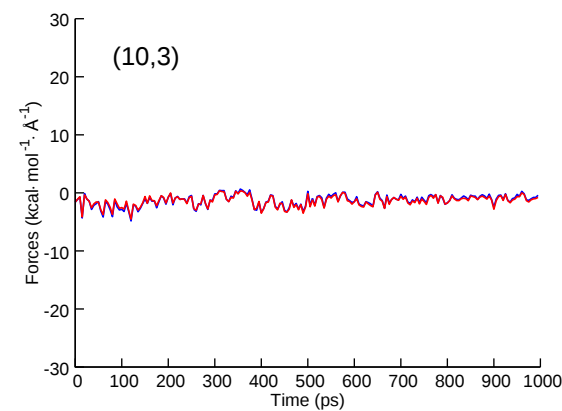
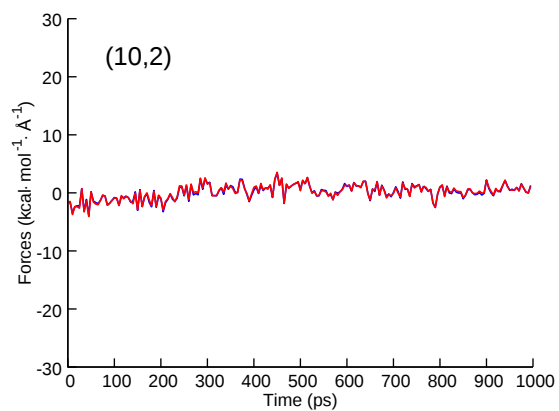
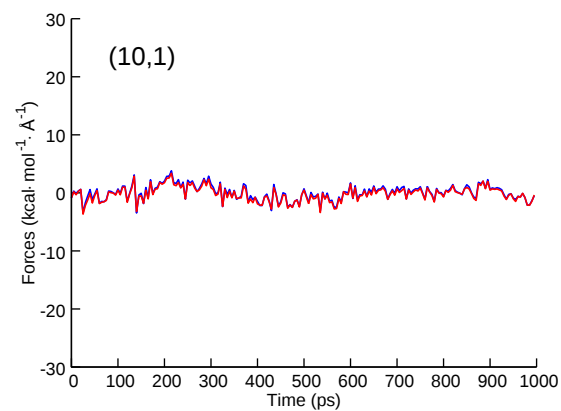


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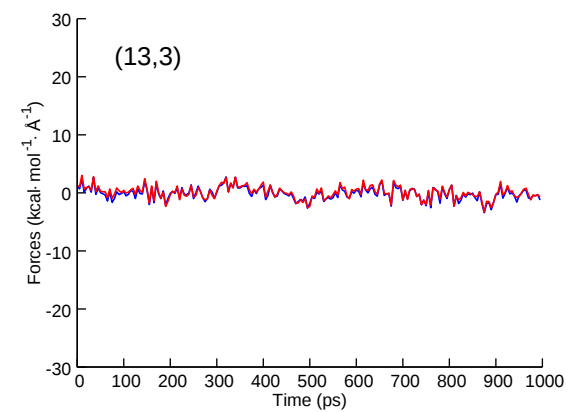
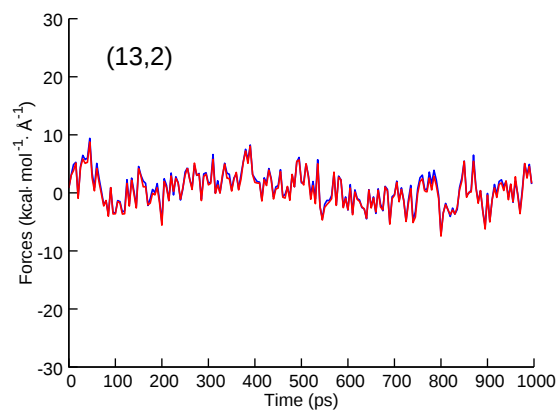
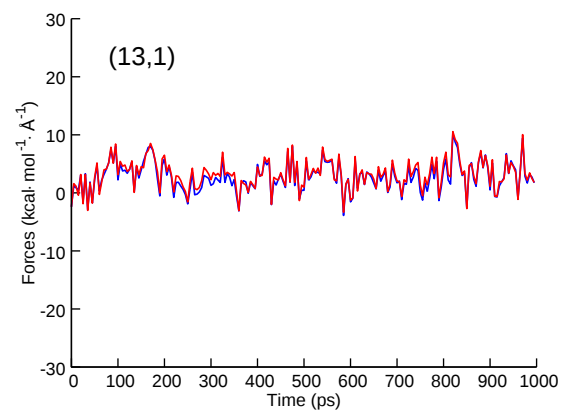


Fig. S4.
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