

ELECTRONIC SUPPLEMENTARY INFORMATION
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**Extended Hamiltonian molecular dynamics: Semiclassical trajectories
with improved maintenance of zero point energy**

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Contents:

Figure S1. The classical and EHMD (with quartic anharmonicity) mode energies as functions of time for quartic system A4 with different κ parameters.	S-2
Figure S2. The classical and EHMD (with quartic anharmonicity) mode energies as functions of time for quartic system A4 with different κ parameters.	S-3
Figure S3. The classical and EHMD (with quartic anharmonicity) mode energies as functions of time for quartic system C4 with different κ parameters.	S-4

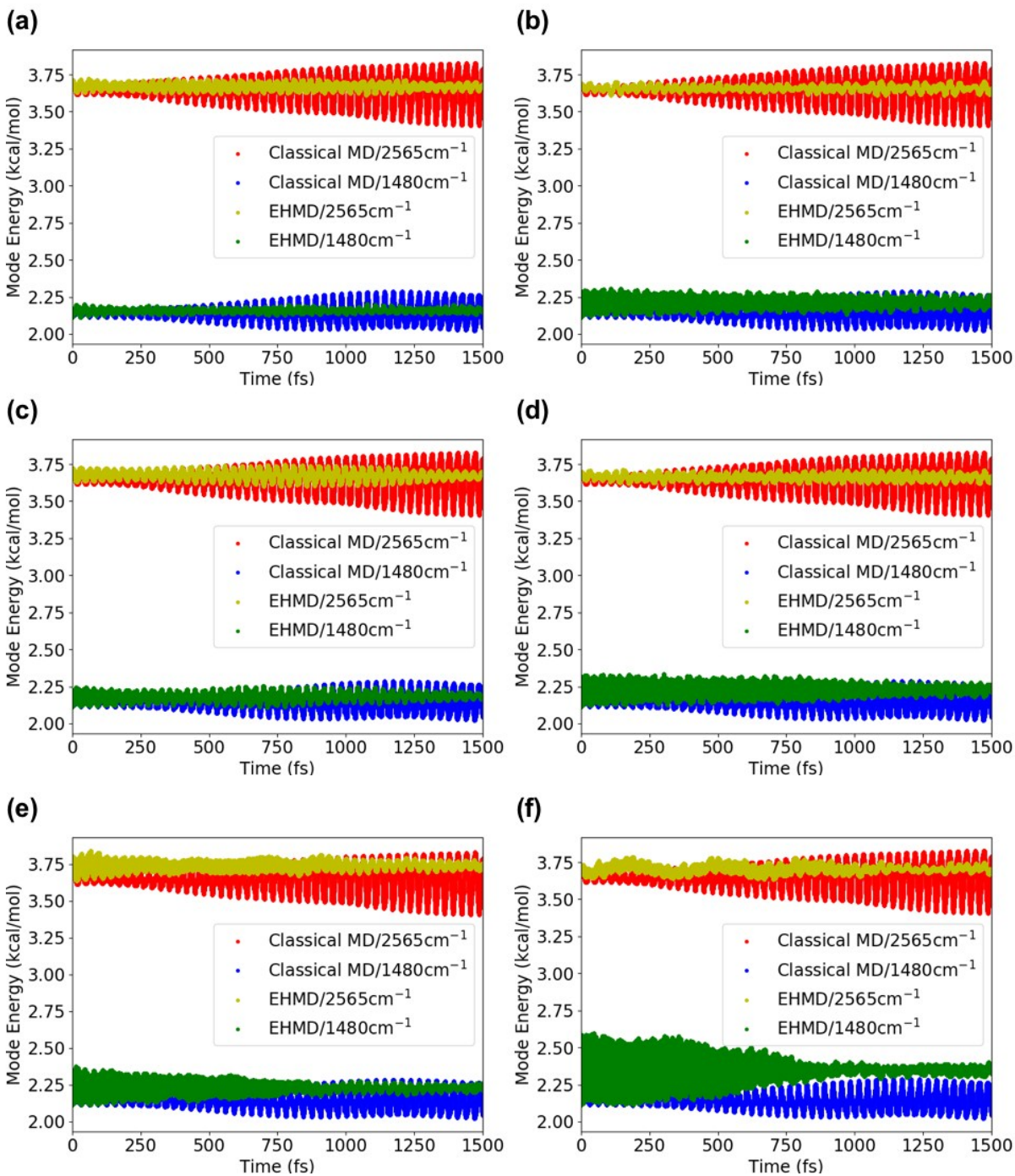


Figure S1. The classical and EHMD (with quartic anharmonicity) mode energies as functions of time for quartic system A4 with different κ parameters. The anharmonic constant λ is set to $0.5(k_1 + k_2)/a_0^2 = 63.717 \text{ N cm}^{-1} \text{ \AA}^{-2}$. The κ values in N cm^{-1} are (a) $\kappa_1 = 2.335$, $\kappa_2 = 0.7784$; (b) $\kappa_1 = 0.7784$, $\kappa_2 = 2.335$; (c) $\kappa_1 = 2.693$, $\kappa_2 = 1.557$; (d) $\kappa_1 = 1.557$, $\kappa_2 = 2.693$; (e) $\kappa_1 = 5.387$, $\kappa_2 = 3.114$; and (f) $\kappa_1 = 3.114$, $\kappa_2 = 5.387$.

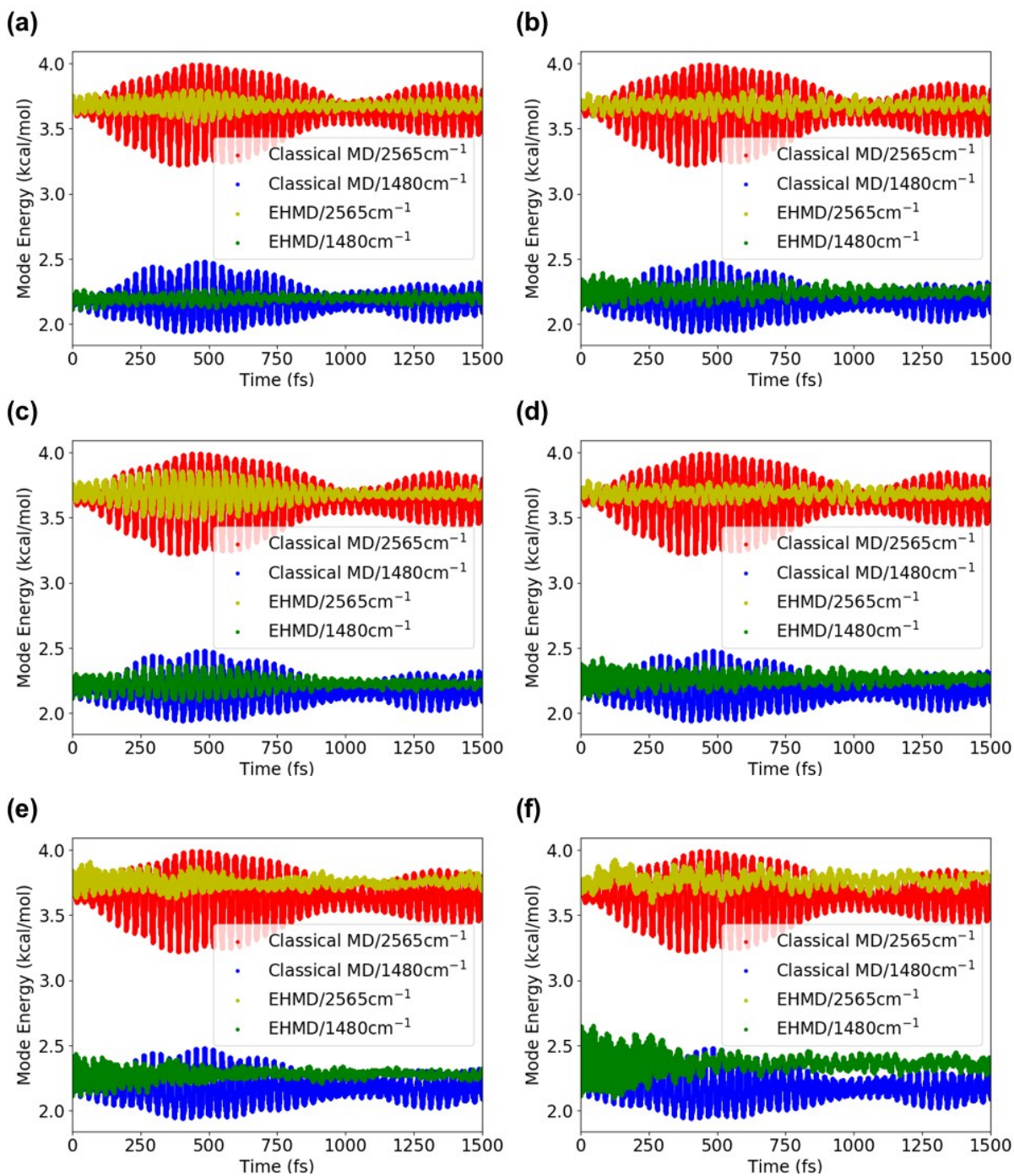


Figure S2. The classical and EHMD (with quartic anharmonicity) mode energies as functions of time for quartic system A4 with different κ parameters. The anharmonic constant λ is set to $(k_1 + k_2)/a_0^2 = 127.434 \text{ N cm}^{-1} \text{ \AA}^{-2}$. The κ values in N cm^{-1} are (a) $\kappa_1 = 2.335$, $\kappa_2 = 0.7784$; (b) $\kappa_1 = 0.7784$, $\kappa_2 = 2.335$; (c) $\kappa_1 = 2.693$, $\kappa_2 = 1.557$; (d) $\kappa_1 = 1.557$, $\kappa_2 = 2.693$; (e) $\kappa_1 = 5.387$, $\kappa_2 = 3.114$; and (f) $\kappa_1 = 3.114$, $\kappa_2 = 5.387$.

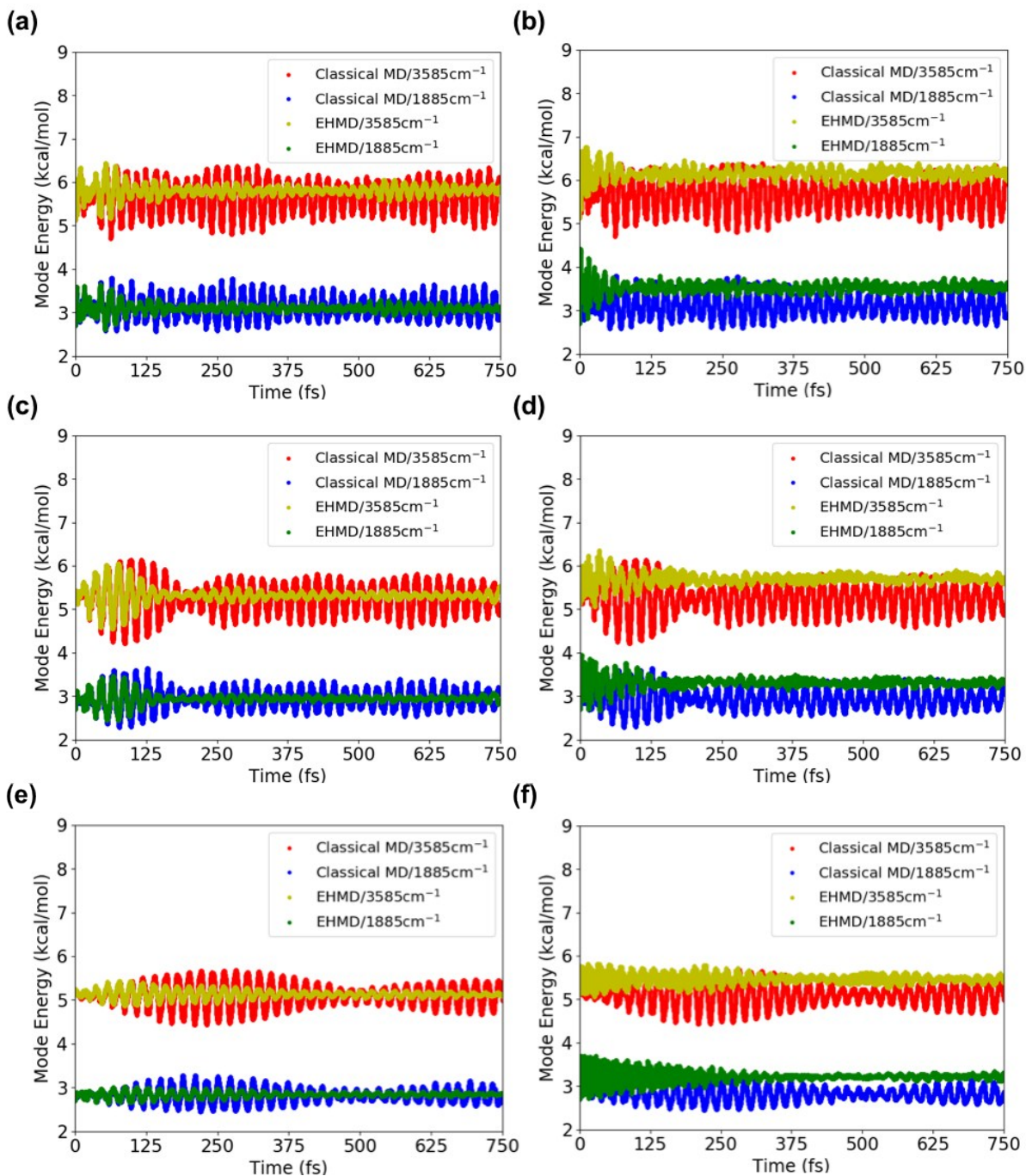


Figure S3. The classical and EHMD (with quartic anharmonicity) mode energies as functions of time for quartic system C4 with different κ parameters. The anharmonic constant λ is set to $(k_1 + k_2)/a_0^2 = 32.720 \text{ N cm}^{-1} \text{ \AA}^{-2}$ for (a) and (b), to $0.5(k_1 + k_2)/a_0^2 = 16.360 \text{ N cm}^{-1} \text{ \AA}^{-2}$ for (c) and (d), and to $0.25(k_1 + k_2)/a_0^2 = 8.180 \text{ N cm}^{-1} \text{ \AA}^{-2}$ for (e) and (f). The κ values in N cm^{-1} are: (a)(c)(e): $\kappa_1 = 0.1479$, $\kappa_2 = 0.07784$; (b)(d)(f): $\kappa_1 = 2.958$, $\kappa_2 = 1.557$.