Supporting Information for: The hole mass in Car-Parrinello molecular dynamics: insights into the dynamics of excitation

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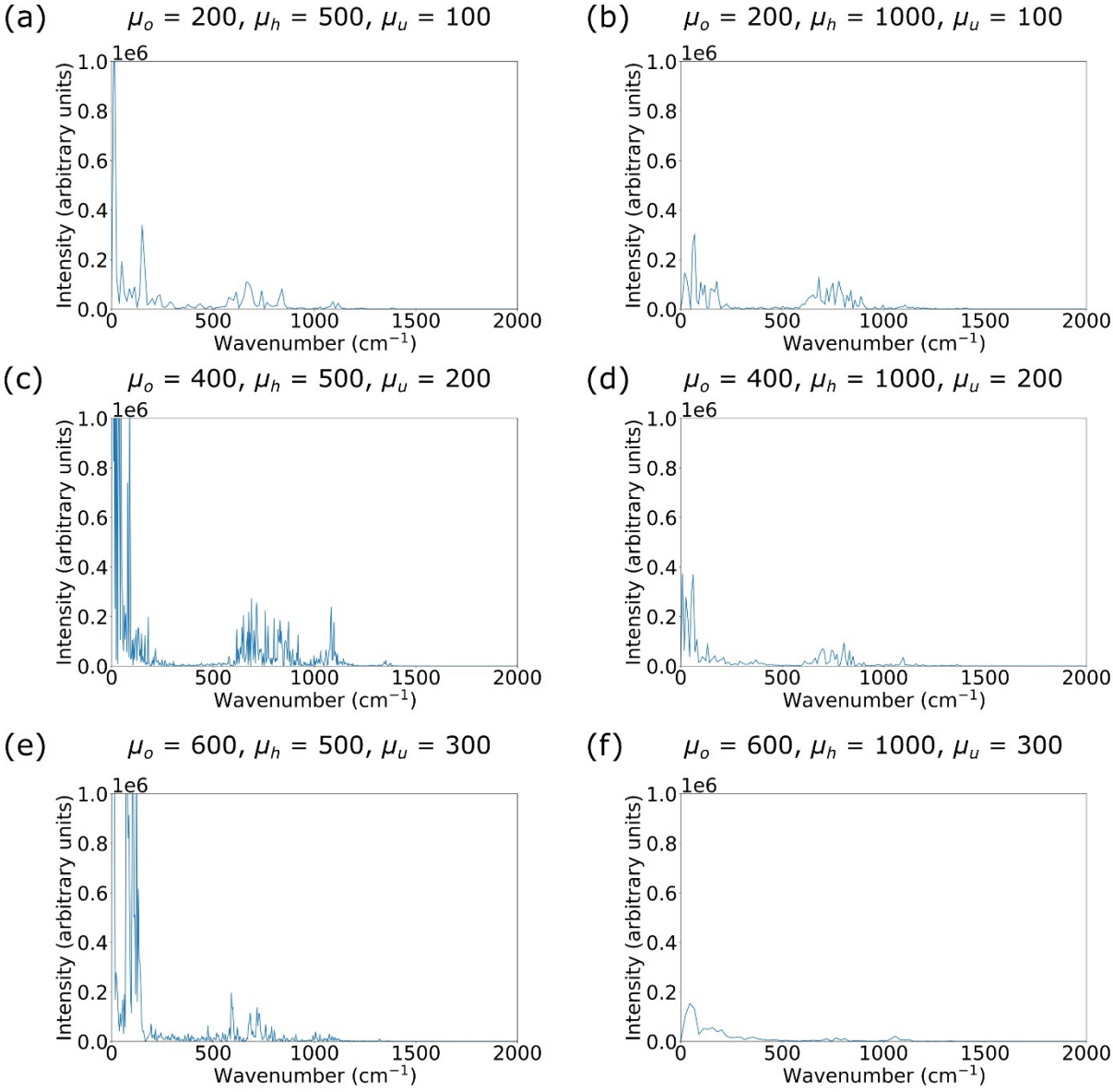

Figure S1: Cyclobutene ring-opening simulations: The Fourier transform of the C3-C4 bond length (Å, $d_{C3\text{-}C4}$) for the six mass values in Table 1: (a) μ_A, (b) μ_B, (c) μ_C, (d) μ_D, (e) μ_E, and (f) μ_F.

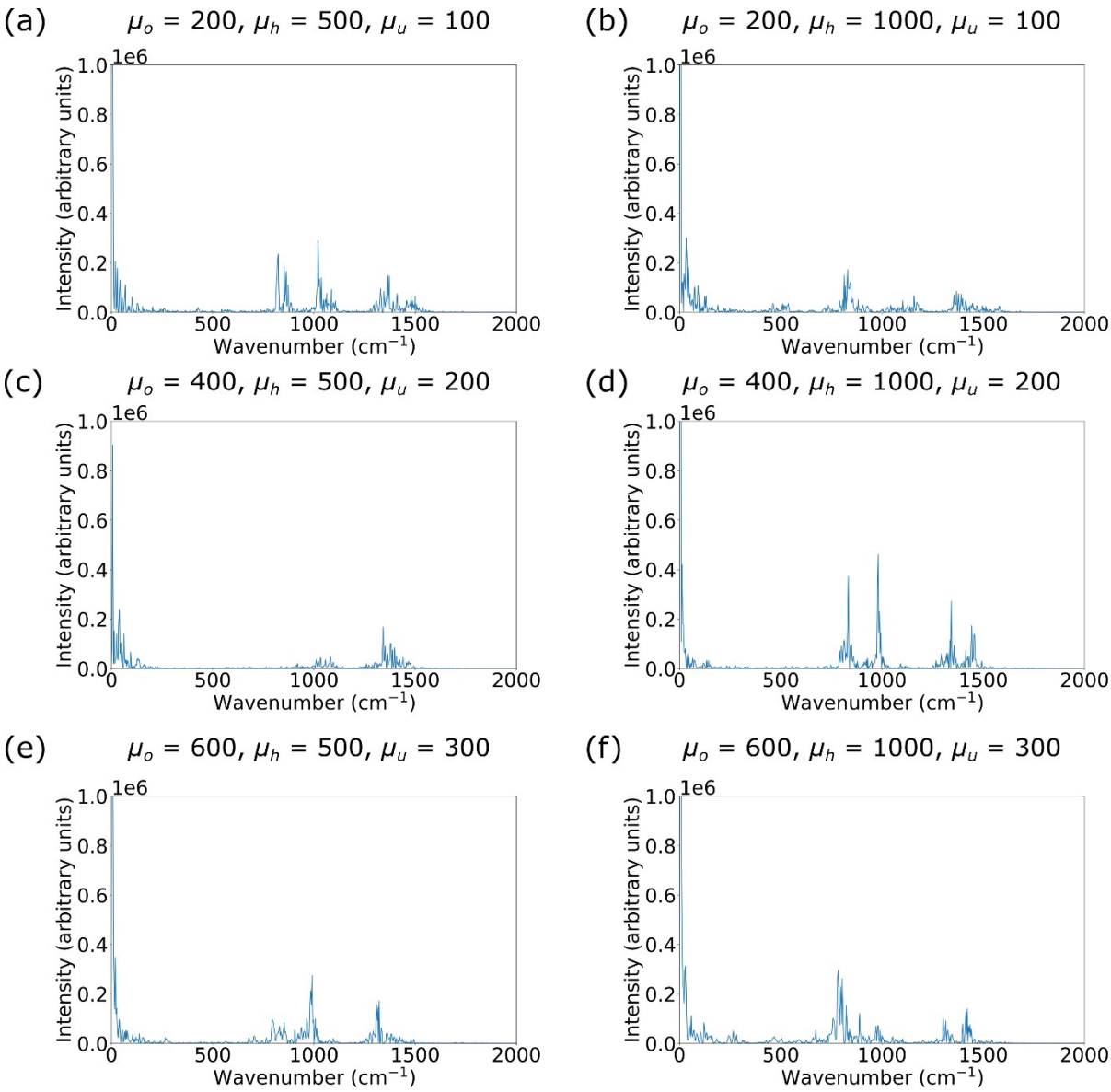

Figure S2: Cyclobutene ring-opening simulations: The Fourier transform of the C1-C2 bond length (Å, $d_{\text{C1-C2}}$) for the six mass values in Table 1: (a) μ_A, (b) μ_B, (c) μ_C, (d) μ_D, (e) μ_E, and (f) μ_F.