Asymmetrical vibrational energy propagation through double or single bonds of small organic molecules. An ab-initio molecular dynamics study

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The present study evaluates the vibrational energy propagation from an O[dbnd]C stretching through the double or single bonds of two small carboxamide molecules. The results show that double bonding facilitates vibrational energy flow while single bonding blockades energy protrusion. Similarly, the direct injection of vibrational energy at a single bond precludes the dissipation of vibrational energy to the rest of the molecular structure generating a vibrational trapping effect. Correlation between bond oscillations and molecular orbital energy fluctuation are analyzed. The presence or absence of those correlations seems to be determinant for vibrational energy flow at the molecular scale.