

GLE type:

GLE options:

Centroid

ω_{\max}

N. beads

Target T

Par. set

Max. physical frequency within range:

$\omega_{\max}=4170.213540000001$ cm⁻¹

Output format:

Paste the relevant lines into the i-PI xml input file.

Efficient sampling of
quasi-classical modes

Rough estimate of the highest
(physical) vibrational mode

Parameters of the PIMD simulation

GLE parameters are fit up to a cutoff frequency...

... pick the parset that gets you closest to the maximum
frequency in your system (veeeery roughly is OK!)