

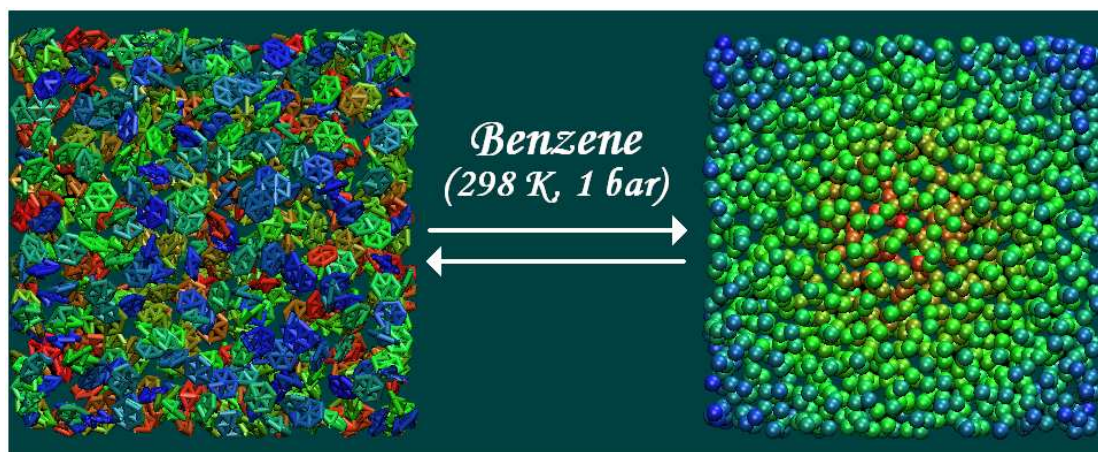
Optimization of coarse-grained interaction potential: inside inherent limitations of coarse-graining methods

Piotr Kowalczyk^{*1}, Piotr A. Gauden² and Alina Ciach³

[1] Nanochemistry Research Institute, Department of Chemistry, Curtin University of Technology, P.O. Box U1987, Perth, 6845 Western Australia, Australia; piotr.kowalczyk@curtin.edu.au

[2] Department of Chemistry, Physicochemistry of Carbon Materials Research Group, N. Copernicus University, Gagarin St. 7, 87-100 Torun, Poland; gaudi@umk.pl

[3] Institute of Physical Chemistry, Polish Academy of Science, Kasprzaka Street 44/52, 01-224 Warsaw, Poland; aciach@ichf.edu.pl



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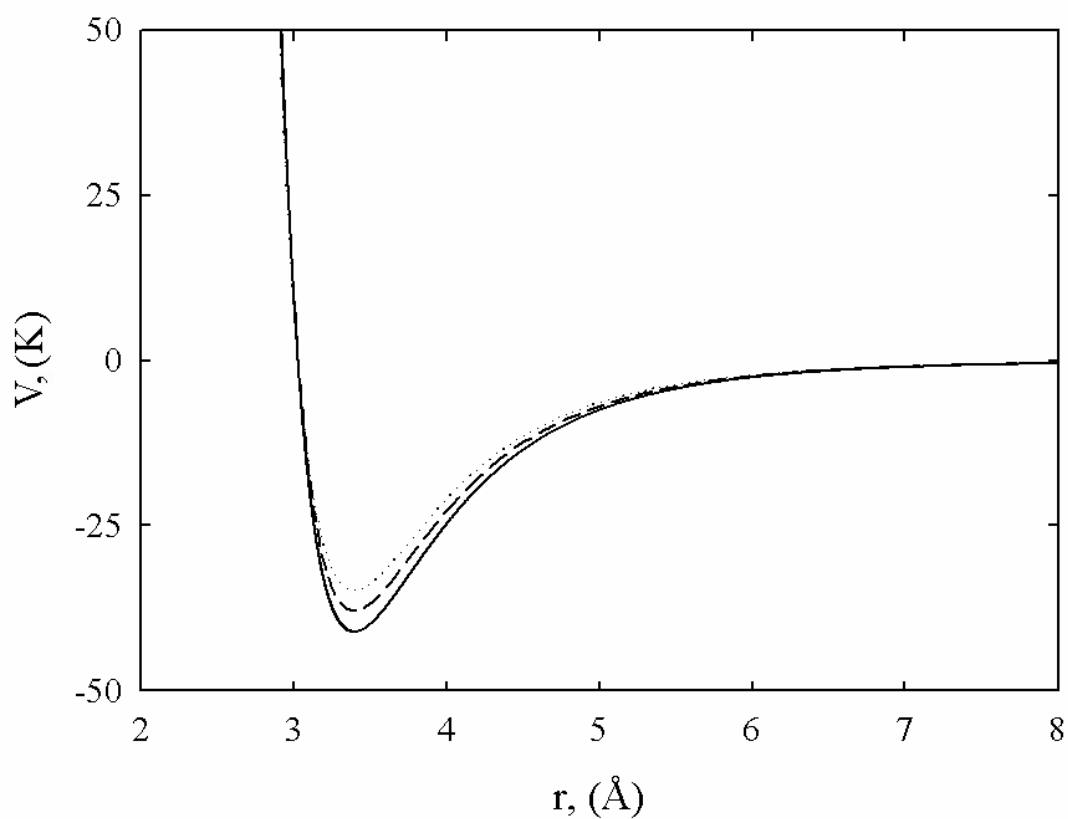


Figure 1S. CG potentials computed for molecular hydrogen at 298 K and 1 bar. Abbreviations: solid line - CG potential optimized for average potential energy per bead, dashed line - optimal CG potential computed from Eq. (5) for $w = 0.5$, and dotted line - CG potential optimized for density.

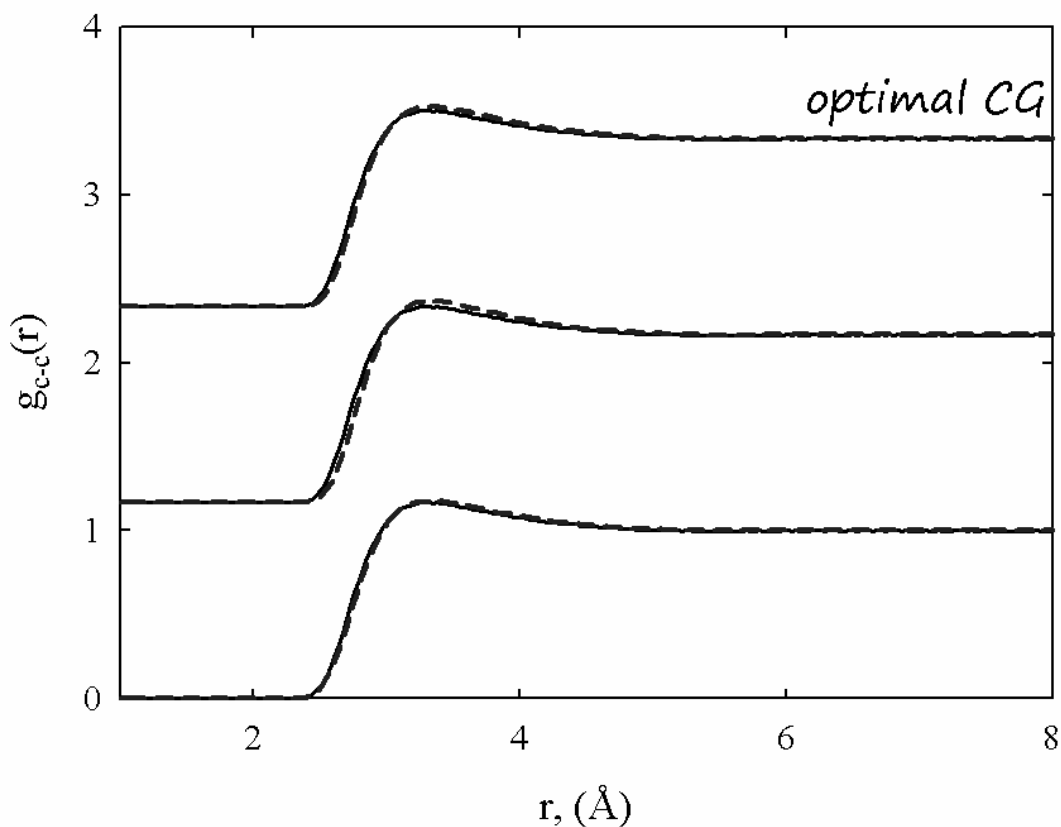


Figure 2S. Radial distribution functions (mass-center-to-mass-center) for molecular hydrogen computed from CG (dashed lines) and atomistic (solid lines) simulation at 298 K and 1 bar. The bottom panel corresponds to CG potential optimized for average potential energy per bead, whereas the middle panel corresponds to CG potential optimized for average density. The upper optimal CG potential is computed from Eq. (5) for $w = 0.5$.

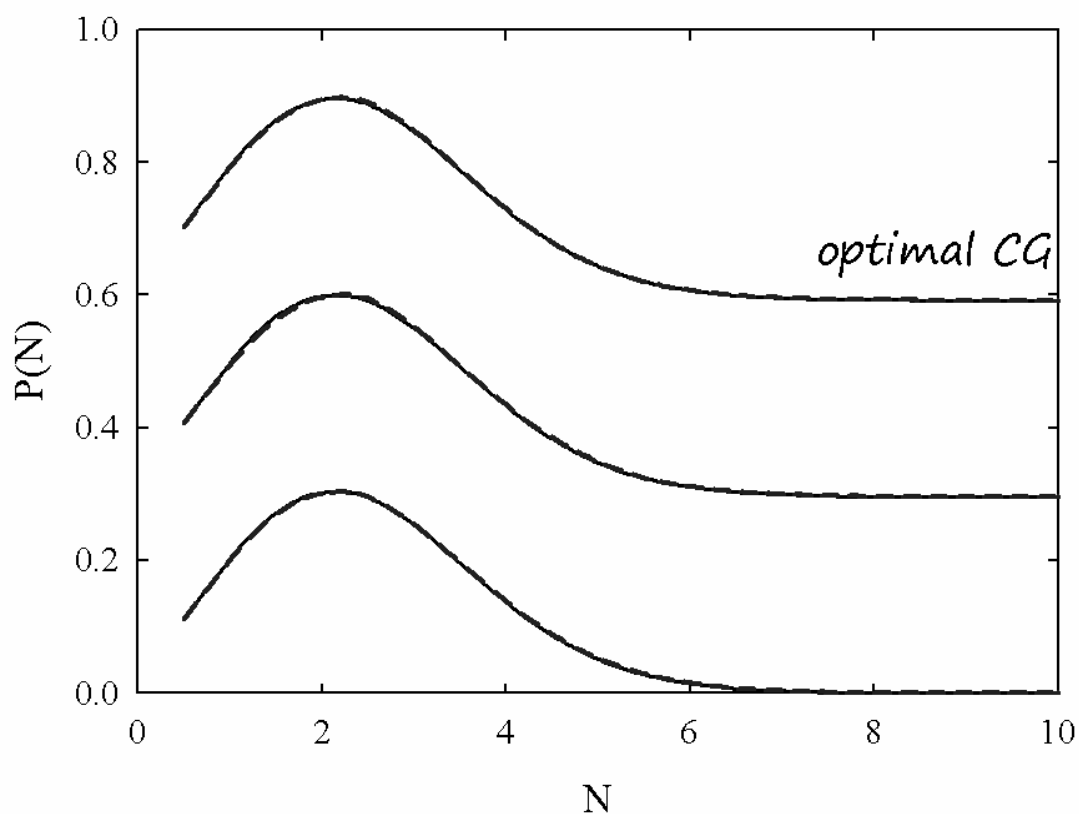


Figure 3S. Probability distributions of the number of hydrogen molecules for the first solvation shell computed from CG (dashed lines) and atomistic (solid lines) simulation of molecular hydrogen at 298 K and 1 bar. The bottom panel corresponds to CG potential optimized for average potential energy per bead, whereas the middle panel corresponds to CG potential optimized for average density. The upper optimal CG potential is computed from Eq. (5) for $w = 0.5$.

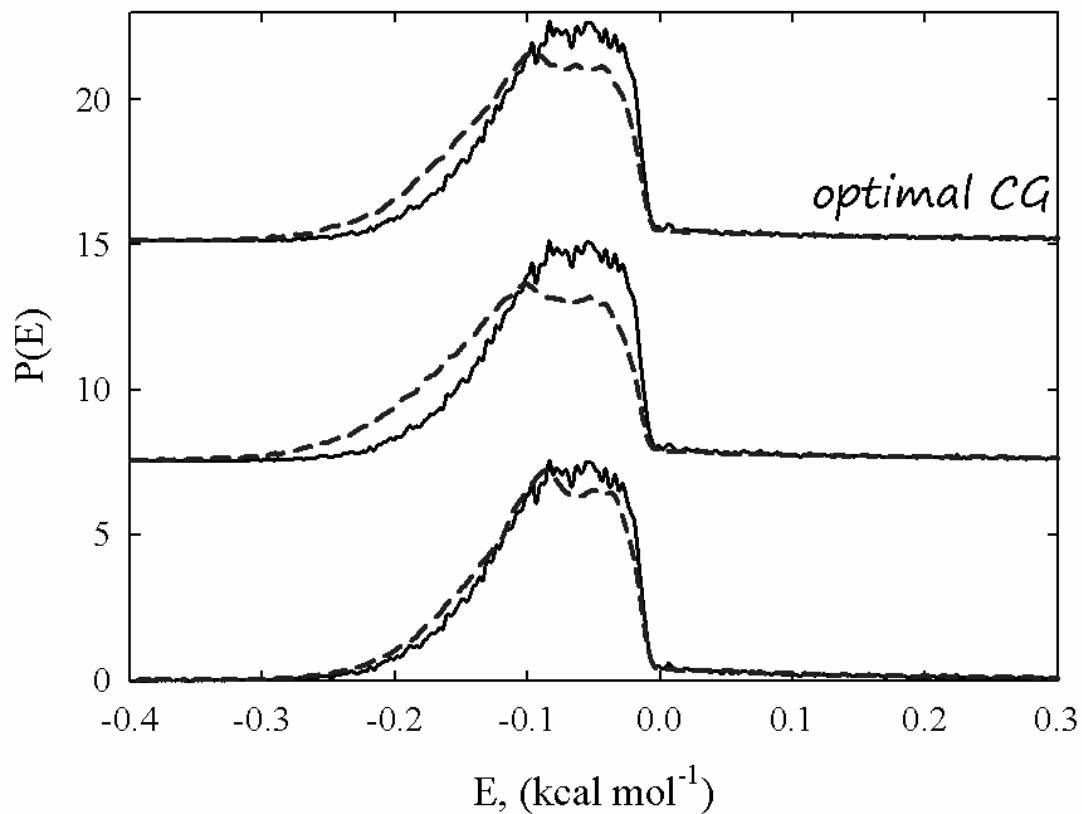


Figure 4S. Distributions of total bonding energies for monomers in molecular hydrogen computed from CG (dashed lines) and atomistic (solid lines) simulation at 298 K and 1 bar. The bottom panel corresponds to CG potential optimized for average potential energy per bead, whereas the middle panel corresponds to CG potential optimized for density. The upper optimal CG potential is computed from Eq. (5) for $w = 0.5$.

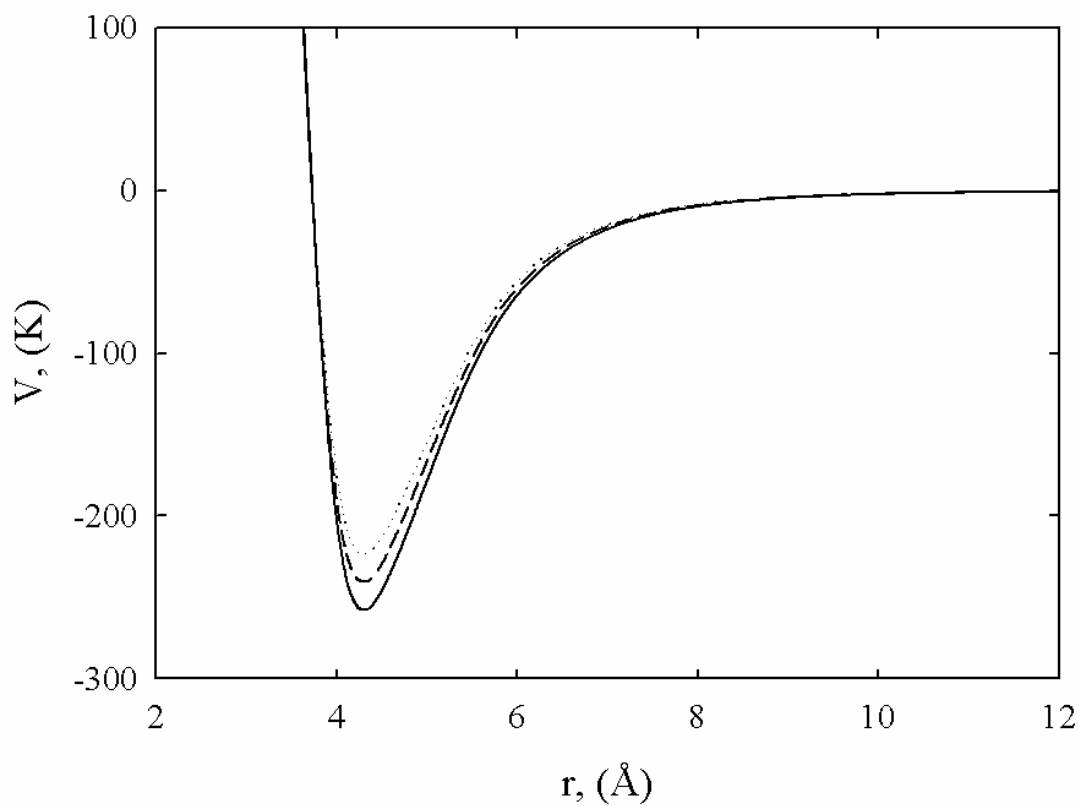


Figure 5S. CG potentials computed for liquid carbon dioxide at 298 K and 1 bar. Abbreviations: solid line - CG potential optimized for average potential energy per bead, dashed line - optimal CG potential computed from Eq. (5) for $w = 0.5$, and dotted line - CG potential optimized for density.

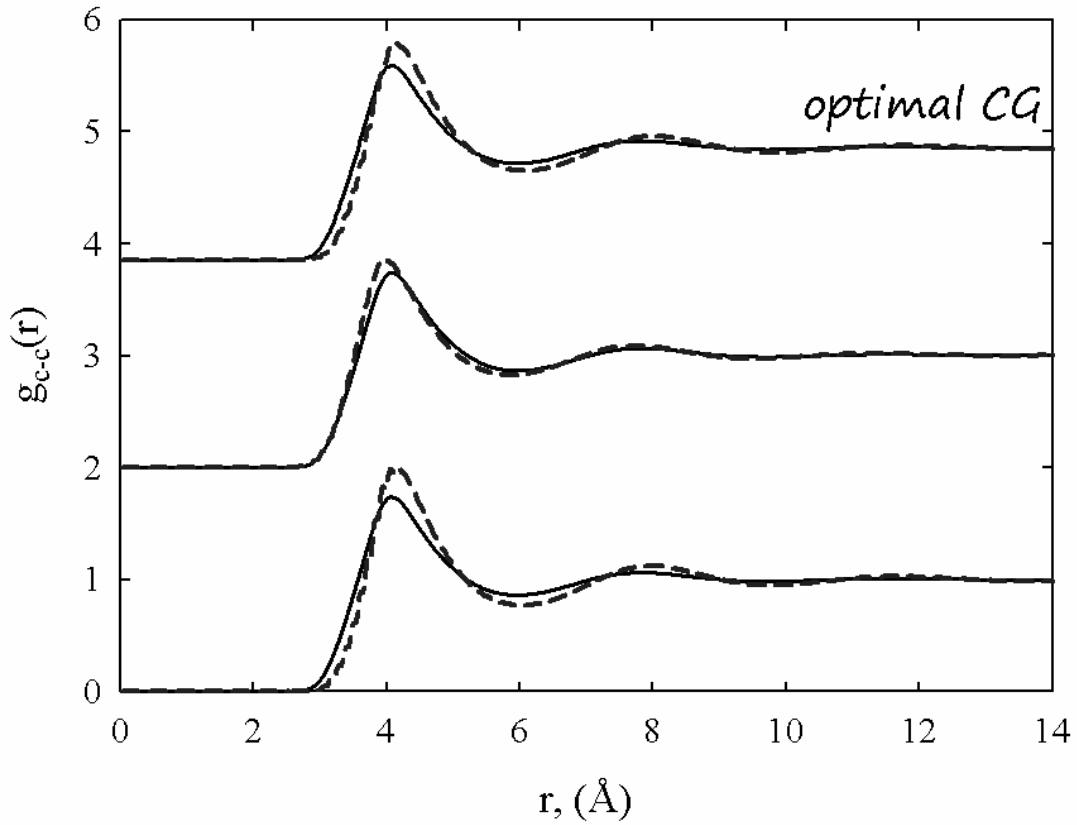


Figure 6S. Radial distribution functions (mass-center-to-mass-center) for liquid carbon dioxide computed from CG (dashed lines) and atomistic (solid lines) simulation at 298 K and 1 bar. The bottom panel corresponds to CG potential optimized for average potential energy per bead, whereas the middle panel corresponds to CG potential optimized for average density. The upper optimal CG potential is computed from Eq. (5) for $w = 0.5$.

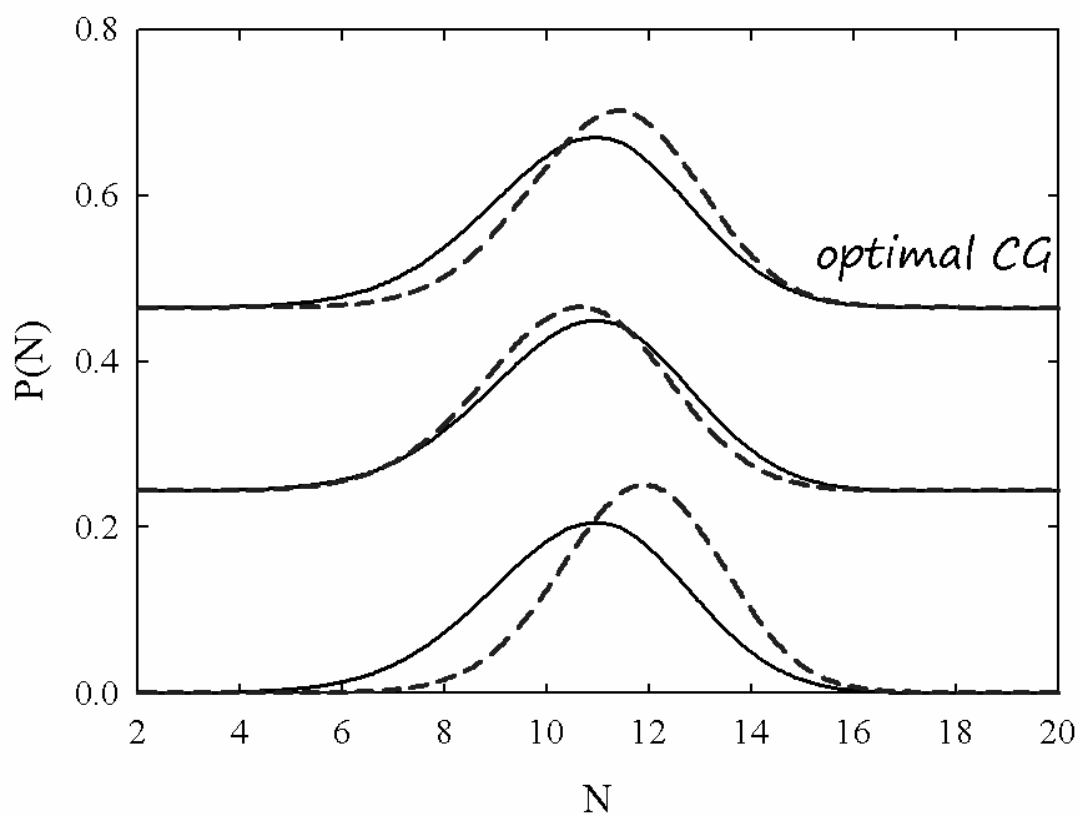


Figure 7S. Probability distributions of the number of carbon dioxide molecules for the first solvation shell computed from CG (dashed lines) and atomistic (solid lines) simulation of liquid carbon dioxide at 298 K and 1 bar. The bottom panel corresponds to CG potential optimized for average potential energy per bead, whereas the middle panel corresponds to CG potential optimized for average density. The upper optimal CG potential is computed from Eq. (5) for $w = 0.5$.

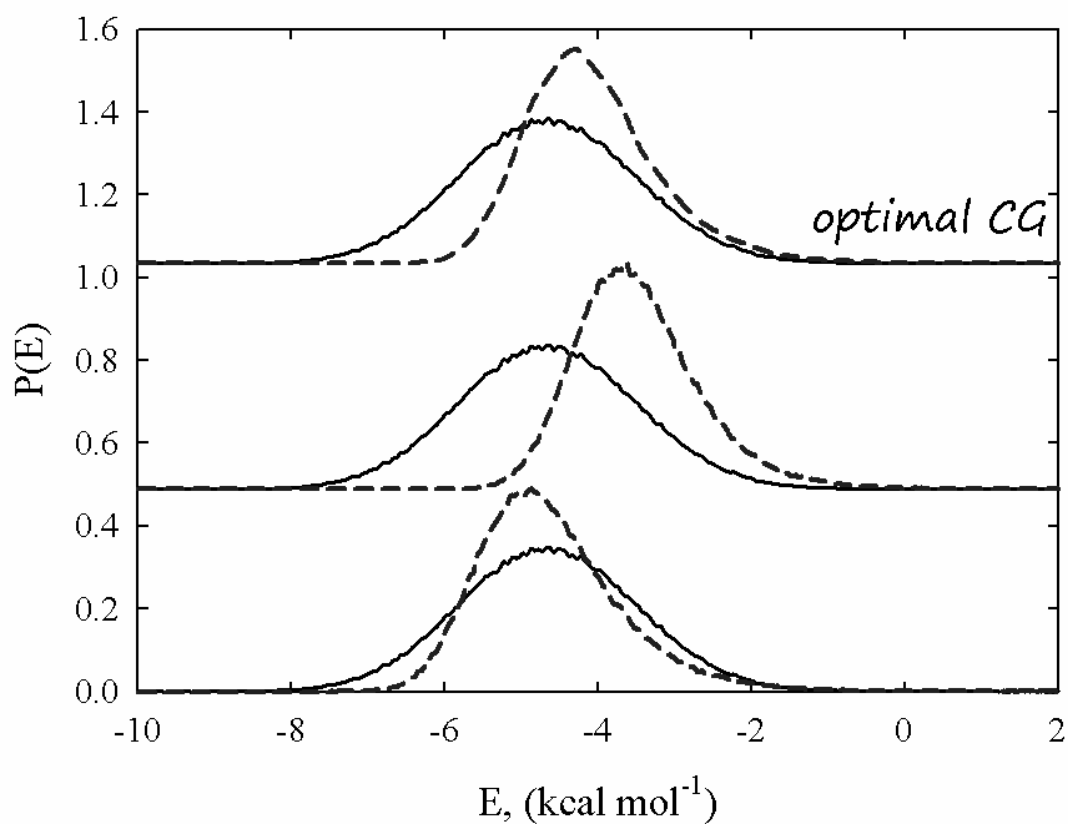


Figure 8S. Distributions of total bonding energies for monomers in liquid carbon dioxide computed from CG (dashed lines) and atomistic (solid lines) simulation at 298 K and 1 bar. The bottom panel corresponds to CG potential optimized for average potential energy per bead, whereas the middle panel corresponds to CG potential optimized for density. The upper optimal CG potential is computed from Eq. (5) for $w = 0.5$.