University of Groningen

Comparison of thermodynamic properties of coarse-grained and atomic-level simulation models

Baron, R.; Trzesniak, D.; de Vries, A.H.; Elsener, A.; Marrink, S.J.; van Gunsteren, W.F.

Published in:
Chemphyschem

DOI:
[10.1002/cphc.200600658](https://doi.org/10.1002/cphc.200600658)

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version
Publisher's PDF, also known as Version of record

Publication date:
2007

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):

Baron, R., Trzesniak, D., de Vries, A. H., Elsener, A., Marrink, S. J., & van Gunsteren, W. F. (2007). Comparison of thermodynamic properties of coarse-grained and atomic-level simulation models. *Chemphyschem*, 8(3), 452 - 461. <https://doi.org/10.1002/cphc.200600658>

Copyright

Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

The publication may also be distributed here under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license. More information can be found on the University of Groningen website: <https://www.rug.nl/library/open-access/self-archiving-pure/taverne-amendment>.

Take-down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from the University of Groningen/UMCG research database (Pure): <http://www.rug.nl/research/portal>. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.

CHEMPHYSCHEM

Supporting Information

© Copyright Wiley-VCH Verlag GmbH & Co. KGaA, 69451 Weinheim, 2007

Supplementary Material

Comparison of Thermodynamic Properties
of Coarse-Grained and Atomic-Level Simulation Models

Riccardo Baron, Daniel Trzesniak, Alex H. de Vries, Andreas Elsener,
Siewert J. Marrink, and Wilfred F. van Gunsteren

Supplementary Tables

TABLE s 1: Hydration free energies of aliphatic hydrocarbons in water from experiments (ΔF_{hyd}^{exp}) and from MD simulation at different model resolutions (ΔF_{hyd}^{CG} and ΔF_{hyd}^{AL}), as displayed in Figure 2. Values from thermodynamic integration (and corresponding errors) are displayed for CG ($r_1 = 0.0$ nm; $r_c = 1.4$ nm) and AL simulations, in the temperature range between 263 and 343 K. All values are in kJ mol^{-1} .

TABLE s 2: Solute-solvent interaction energy change upon hydration (ΔU_{uv}) for C4, C8, C12 and C16 in water, as displayed in Figure 3. Values from thermodynamic integration (and corresponding errors) are displayed for CG ($r_1 = 0.0$ nm; $r_c = 1.4$ nm) and AL simulations, in the temperature range between 263 and 343 K. All values are in kJ mol^{-1} .

TABLE s 3: Solvent-solute entropy change upon hydration (ΔS_{uv}) for C4, C8, C12 and C16 in water, as displayed in Figure 4. Values from thermodynamic integration (and corresponding errors) are displayed for CG CG ($r_1 = 0.0$ nm; $r_c = 1.4$ nm) and AL simulations, in the temperature range between 263 and 343 K. All values are in $\text{J mol}^{-1} \text{K}^{-1}$.

TABLE s 1:

	$\Delta F_{hyd}^{exp, a}$	ΔF_{hyd}^{CG} and $\Delta F_{hyd}^{AL, b}$									
	298 K	263 K		283 K		303 K		323 K		343 K	
		CG	AL	CG	AL	CG	AL	CG	AL	CG	AL
<i>n</i> -butane	9.0	10.1 (0.3)	6.4 (0.9)	11.9 (0.3)	8.5 (0.8)	13.7 (0.3)	9.6 (0.8)	15.3 (0.3)	10.0 (0.9)	16.9 (0.3)	10.9 (0.9)
<i>n</i> -octane	12.1	13.6 (0.4)	6.6 (1.7)	16.5 (0.4)	9.0 (1.5)	19.8 (0.4)	11.9 (1.5)	22.8 (0.5)	12.1 (1.7)	25.5 (0.5)	14.3 (1.8)
<i>n</i> -dodecane	---	19.3 (0.6)	8.5 (1.7)	24.8 (0.5)	12.0 (1.7)	29.4 (0.5)	17.9 (1.7)	34.1 (0.5)	18.3 (1.7)	38.5 (0.6)	21.0 (1.8)
<i>n</i> -hexadecane	---	24.7 (0.6)	10.9 (2.4)	30.5 (0.6)	14.7 (2.3)	36.9 (0.5)	19.7 (2.0)	43.5 (0.6)	21.6 (2.0)	48.2 (0.6)	25.9 (1.8)

[a] Experimental values taken from Ben-Naim and Marcus 1987.

[b] Calculated values are for N,V,T ensembles as described in the Computational Methods section. Volumes were different for each system and each temperature as obtained after equilibration at constant pressure.

TABLE s 2:

	ΔU_{uv}^{CG} and ΔU_{uv}^{AL}									
	263 K		283 K		303 K		323 K		343 K	
	CG	AL	CG	AL	CG	AL	CG	AL	CG	AL
<i>n</i> -butane	-15.7 (0.3)	-38.6 (3.9)	-15.4 (0.3)	-37.7 (4.0)	-15.0 (0.4)	-35.6 (4.3)	-14.6 (0.4)	-35.2 (4.4)	-14.2 (0.4)	-33.5 (4.6)
<i>n</i> -octane	-29.5 (0.4)	-68.2 (5.1)	-29.0 (0.4)	-65.6 (5.2)	-28.6 (0.4)	-63.9 (5.4)	-28.0 (0.5)	-61.7 (5.6)	-27.4 (0.5)	-58.8 (6.0)
<i>n</i> -dodecane	-43.2 (0.5)	-97.1 (6.0)	-42.7 (0.5)	-94.4 (6.7)	-42.1 (0.5)	-90.4 (7.0)	-41.4 (0.5)	-87.1 (6.8)	-40.7 (0.6)	-84.3 (7.2)
<i>n</i> -hexadecane	-56.9 (0.5)	-126.8 (6.9)	-56.2 (0.6)	-122.6 (7.4)	-55.6 (0.6)	-115.0 (7.8)	-54.9 (0.6)	-112.2 (7.9)	-54.1 (0.7)	-108.1 (8.4)

TABLE s 3:

	ΔS_{uv}^{CG} and ΔS_{uv}^{AL}									
	263 K		283 K		303 K		323 K		343 K	
	CG	AL	CG	AL	CG	AL	CG	AL	CG	AL
<i>n</i> -butane	-98 (1)	-171 (18)	-96 (1)	-163 (18)	-95 (1)	-149 (17)	-92 (1)	-140 (16)	-91 (1)	-129 (16)
<i>n</i> -octane	-164 (1)	-284 (26)	-161 (1)	-264 (24)	-160 (1)	-250 (23)	-157 (1)	-228 (23)	-154 (1)	-213 (23)
<i>n</i> -dodecane	-238 (1)	-401 (29)	-238 (1)	-376 (30)	-236 (1)	-357 (29)	-234 (1)	-326 (26)	-231 (1)	-307 (26)
<i>n</i> -hexadecane	-310 (1)	-523 (35)	-306 (1)	-485 (34)	-305 (1)	-444 (32)	-305 (1)	-414 (30)	-298 (1)	-391 (30)

Supplementary Figures

Figure s 1: Free energy derivative of removing C4 from water for (a) CG or (b) AL simulations. $\langle \partial H / \partial \lambda \rangle$ values and their errors are shown from simulations at 263 K (cyan), 283 K (green), 303 K (black), 323 K (orange), and 343 K (red). The error bars have been estimated from block averaging. Simulation times per λ -point ranged from 3 to 15 ns (CG) or from 0.2 to 6 ns (AL).

Figure s 2: Solvent-solvent (reorganization) entropy change upon hydration (ΔS_{vv}) as a function of the simulation reference temperature for CG (empty circles) and AL (filled circles) simulations of (a) C4, (b) C8, (c) C12 and (d) C16.

Figure s 3: Lennard-Jones potential energy functions as defined and implemented in GROMOS05^[51] (black line) and as defined (but not implemented) in the GROMACS manuals^[50] (dashed line). The energy is displayed in the sample case of the interaction between two CG water beads as a function of their distance.

Figure s 1:

Figure s 2:

Figure s 3: