ELECTRONIC SUPPLEMENTARY INFORMATION

Toward realistic computer modeling of paraffin-based composite materials: Critical assessment of atomic-scale models of paraffins

Artyom D. Glova,[1] Igor V. Volgin,[1] Victor M. Nazarychev,[1] Sergey V. Larin,[1] Sergey V. Lyulin[1,2] and Andrey A. Gurtovenko[*,1,2]

[1]Institute of Macromolecular Compounds, Russian Academy of Sciences, Bolshoi Prospect V.O. 31, St.Petersburg, 199004, Russia
[2]Faculty of Physics, St. Petersburg State University, Ulyanovskaya Street 3, Petrodvorets, St.Petersburg, 198504, Russia

E-mail: a.gurtovenko@gmail.com

Table S1. Computational performance of 10 considered force fields in molecular dynamics simulations of n-eicosane samples at T = 450K in the NVT ensemble. All simulations were carried out on 70 cores (Intel Xeon CPU E5-2697 v3 (2.60 GHz)) of the Lomonosov-2 supercomputer. United-atom models are much faster than their all-atom counter-parts due to a smaller system size (20,000 vs 60,000 atoms) as well as zero partial charges (the united-atom models of eicosane do not require calculations of electrostatic interactions). The force field-specific cut-off radius of the van der Waals interactions also matters.

Force field	Performance, ns/day
GAFF2	85.7±0.4
GAFF	83.6±0.4
CHARMM36	52.4±0.1
L-OPLS-AA	47.4±0.2
OPLS-AA	46.9±0.2
PYS	693.4±0.9
NERD	556.3±4.8
GROMOS	463.6±3.5
TraPPE	443.1±1.3
OPLS-UA	395.9±0.2

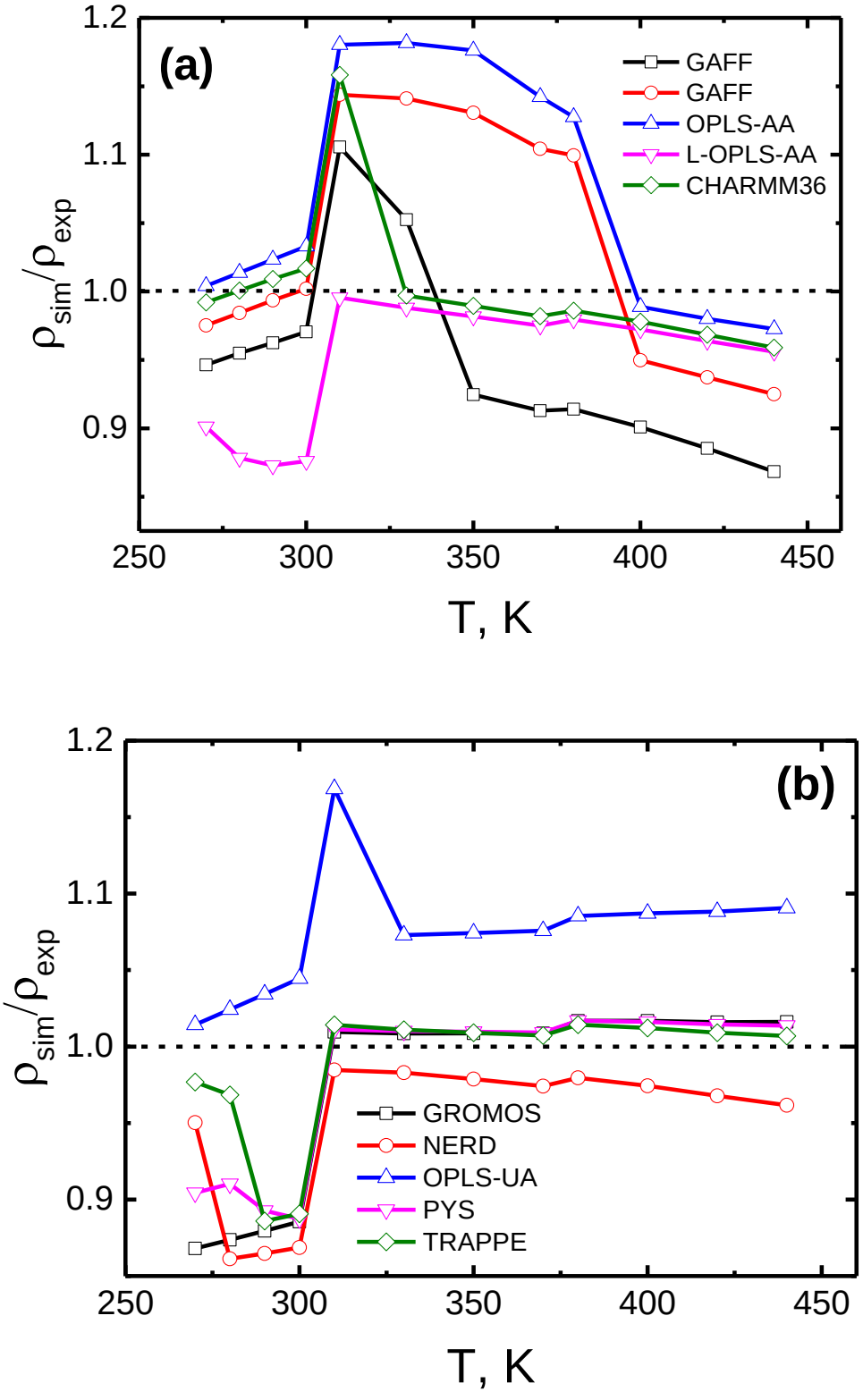

Fig. S1. The ratio ρ_{sim}/ρ_{exp} between computational and experimental[1] values of density of n-eicosane samples as a function of temperature. Shown are results for all-atom (a) and united-atom (b) force fields.

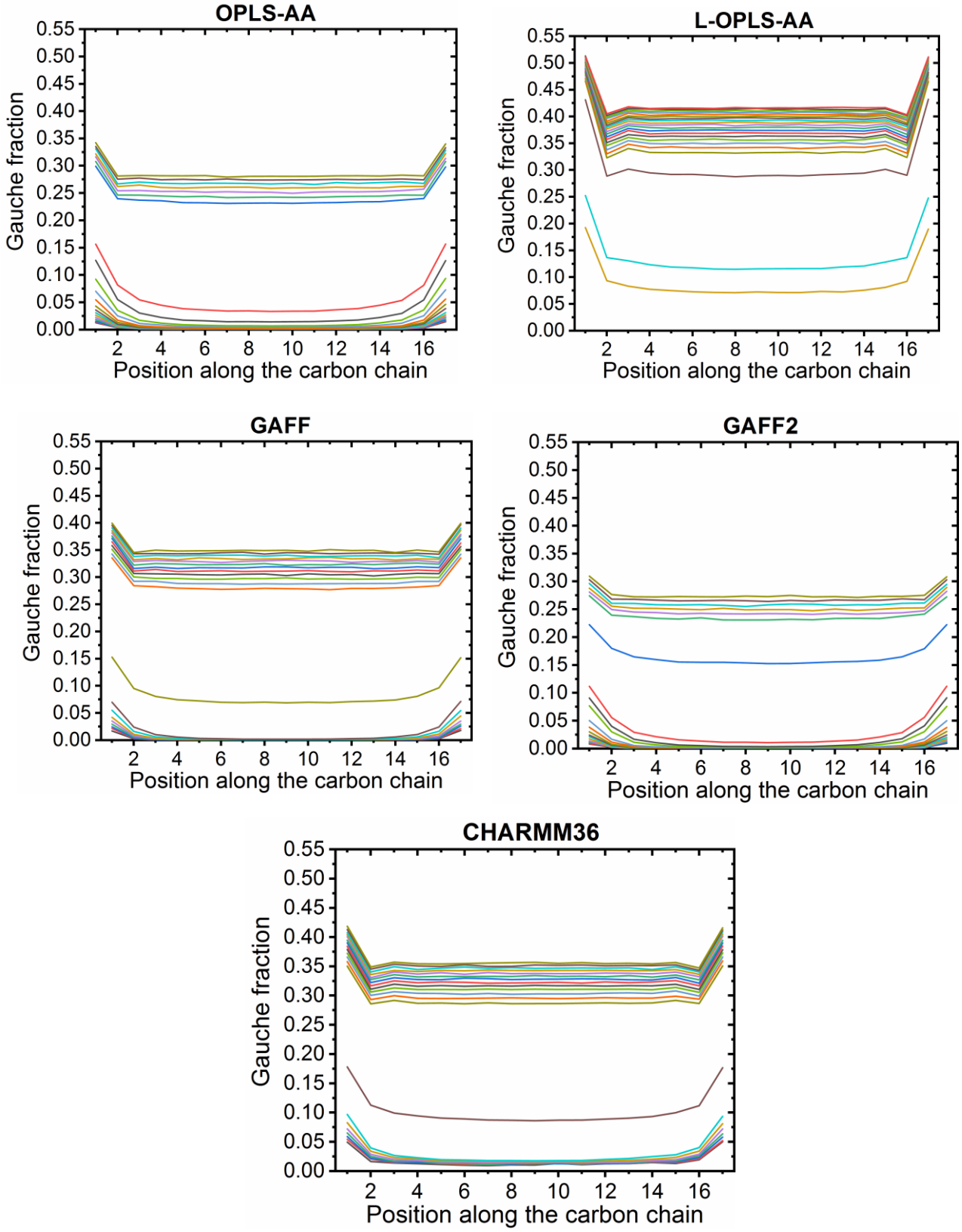

Fig. S2. Fractions of gauche conformers along the hydrocarbon chain for all-atom force fields in the temperature range from 250 to 450 K. Positions of curves become lower with decreasing temperature.

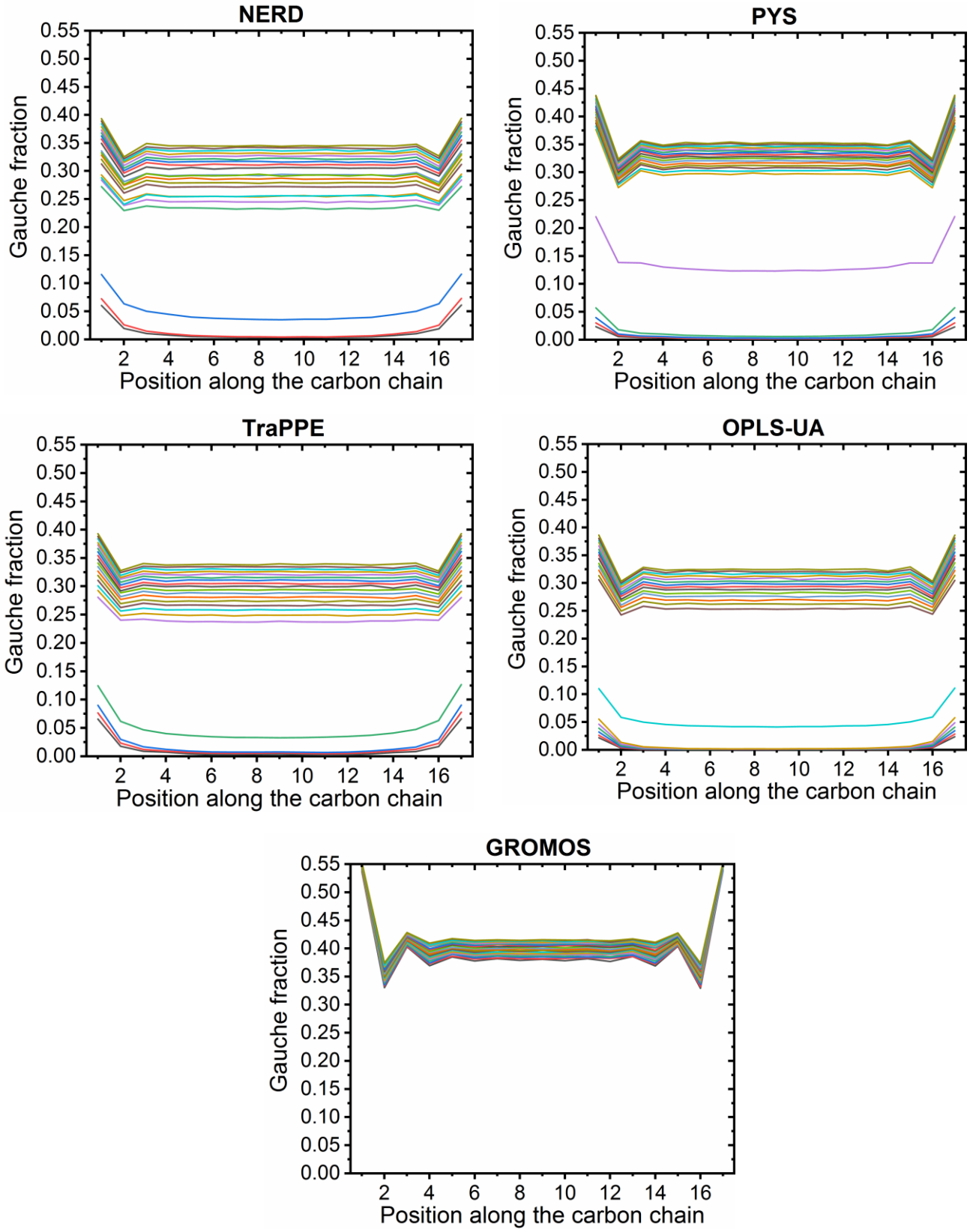

Fig. S3. Fractions of gauche conformers along the hydrocarbon chain for united-atom force fields in the temperature range from 250 to 450 K. Positions of curves become lower with decreasing temperature.

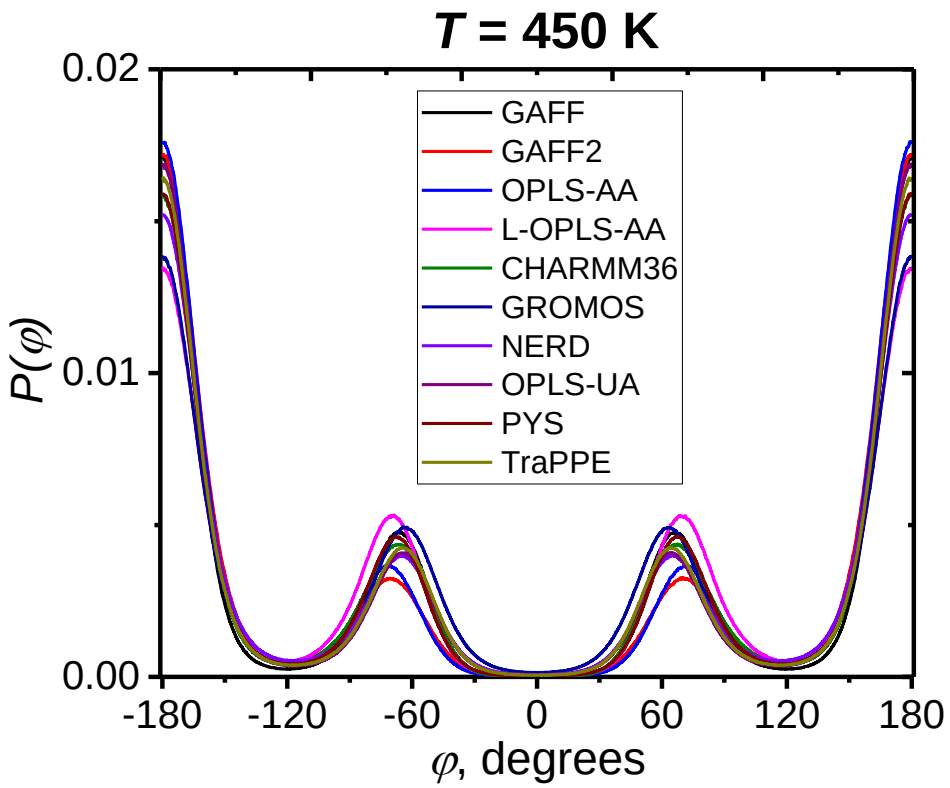

Fig. S4. The probability distribution of the dihedral angle φ for different force fields at T = 450 K.

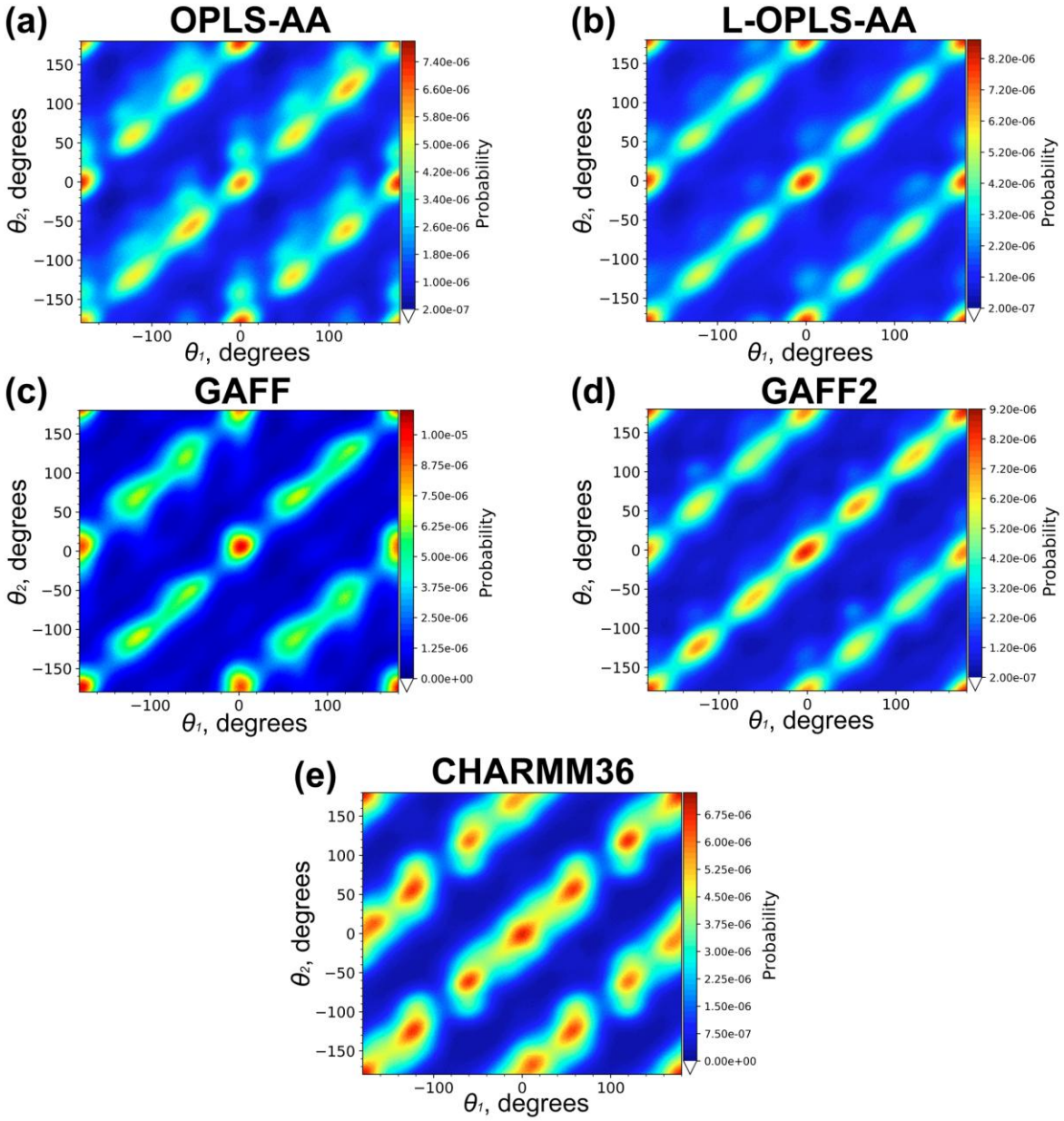

Fig. S5. The probability distribution $P(\theta_1,\theta_2)$ for the n-eicosane crystalline phase simulated with the use of all-atom models. Show are results for configuration 2.

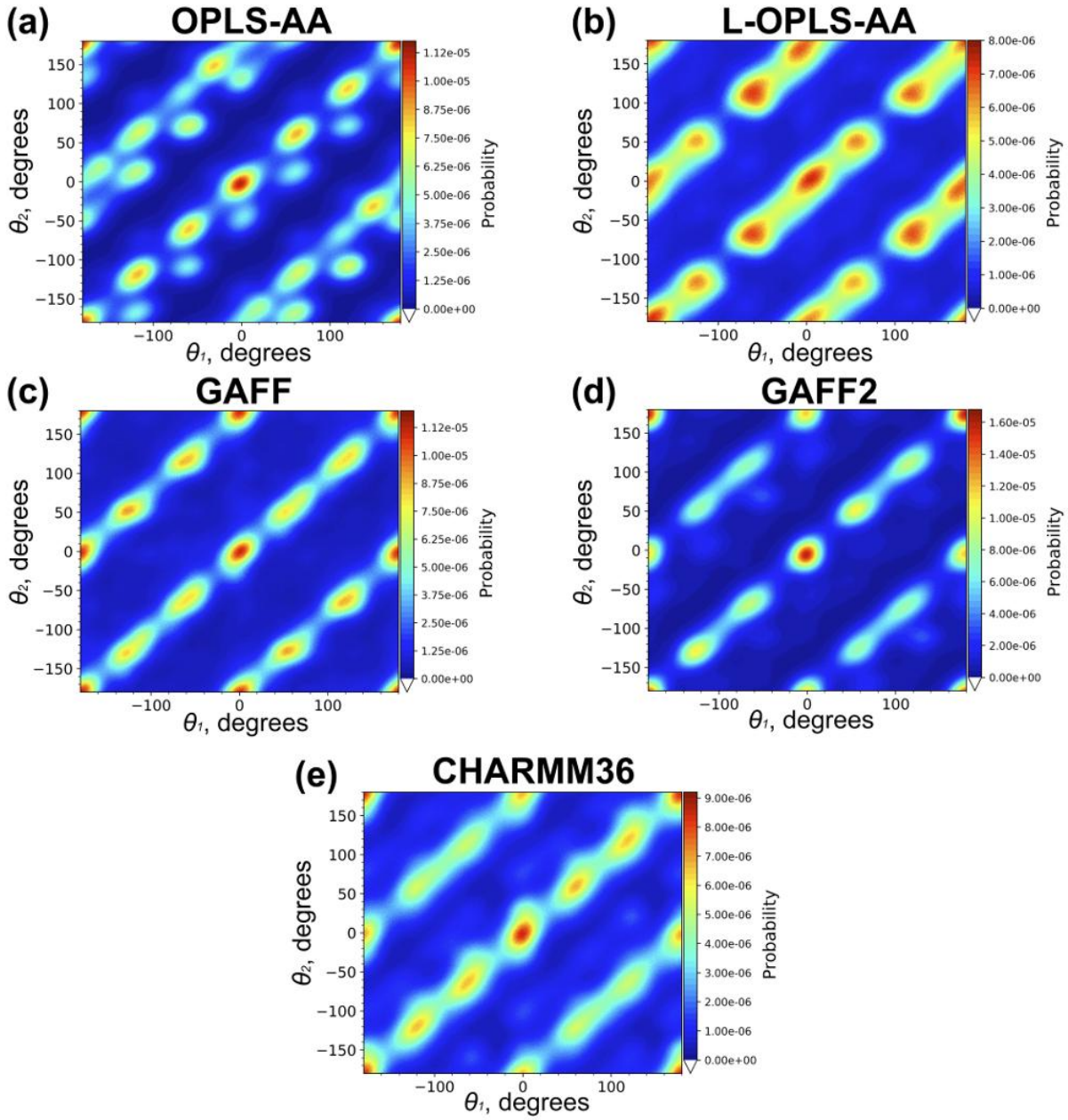

Fig. S6. The probability distribution $P(\theta_1,\theta_2)$ for the n-eicosane crystalline phase simulated with the use of all-atom models. Show are results for configuration 3.

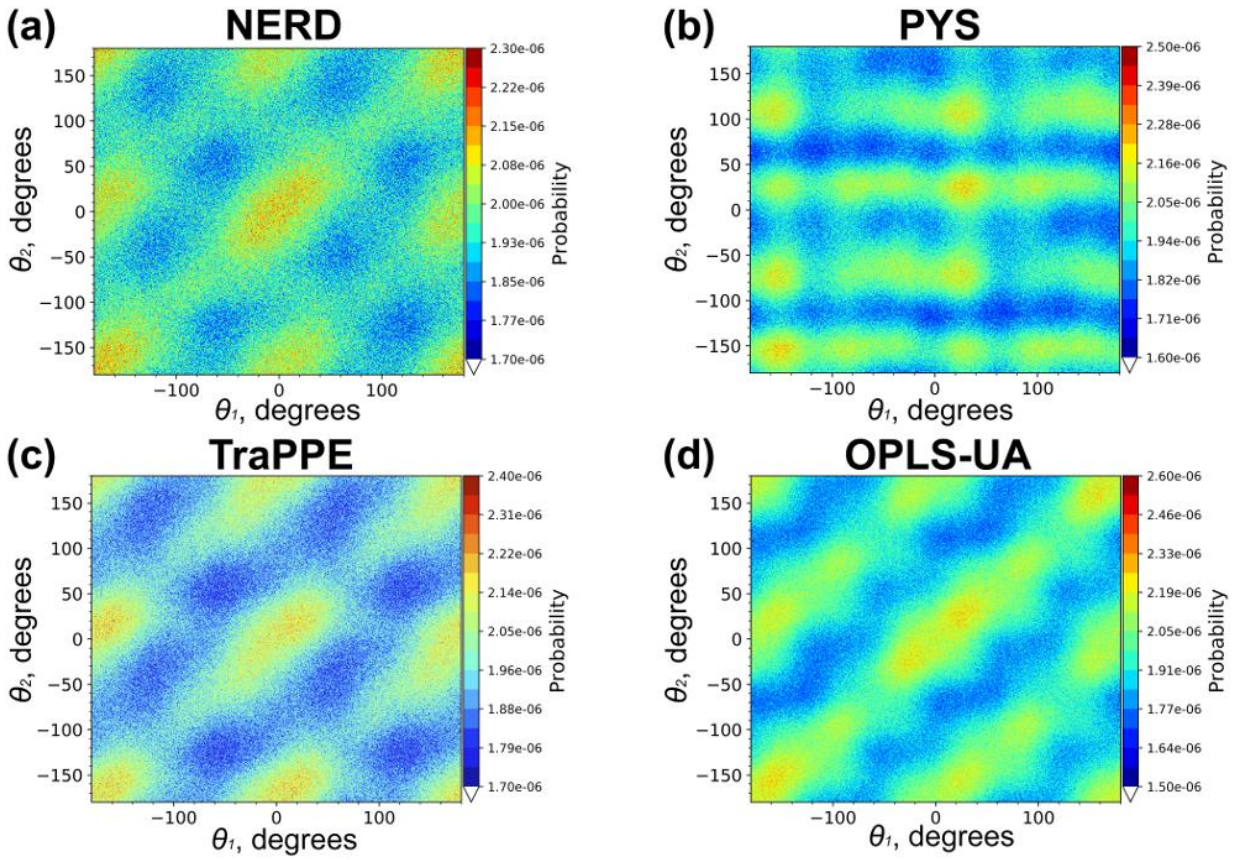

Fig. S7. The probability distribution $P(\theta_1,\theta_2)$ for the n-eicosane crystalline phase simulated with the use of united-atom models. Show are results for configuration 2.

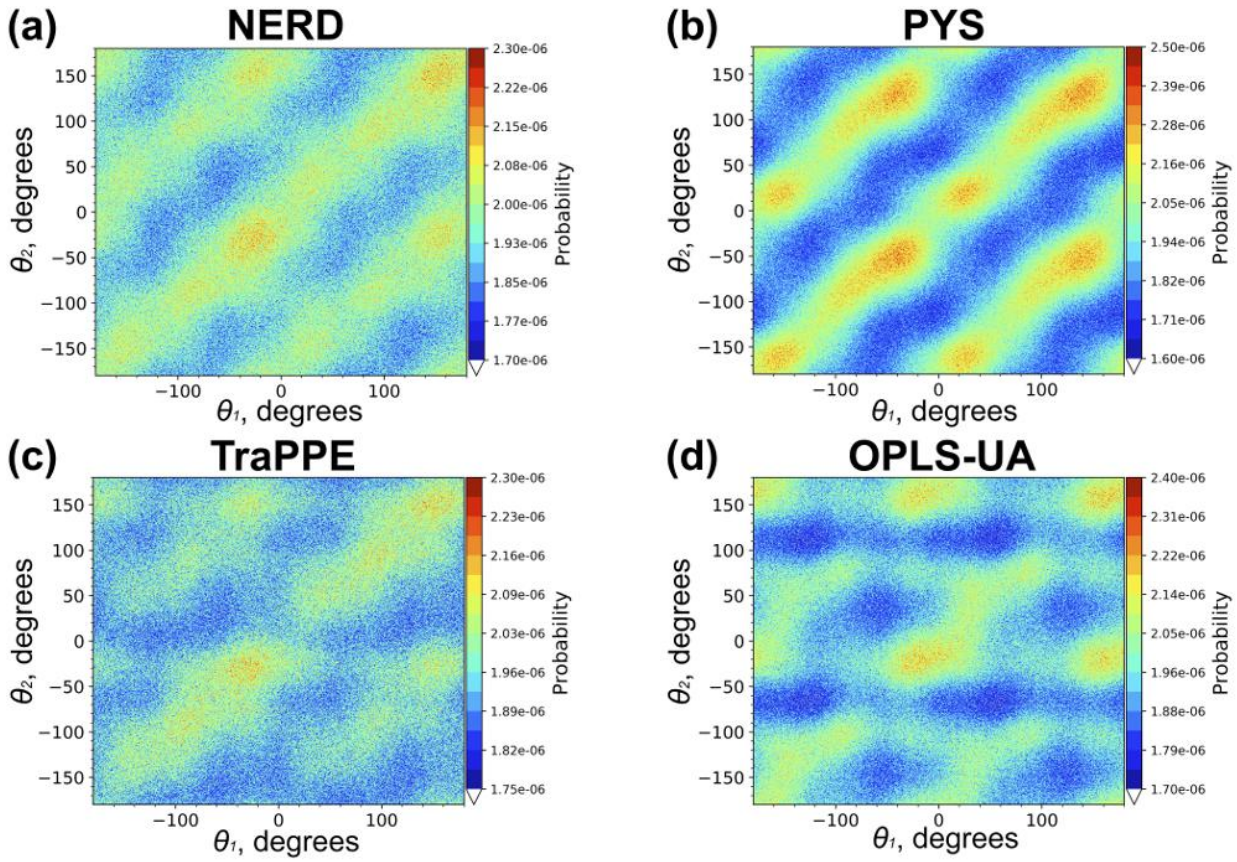

Fig. S8. The probability distribution $P(\theta_1,\theta_2)$ for the n-eicosane crystalline phase simulated with the use of united-atom models. Show are results for configuration 3.

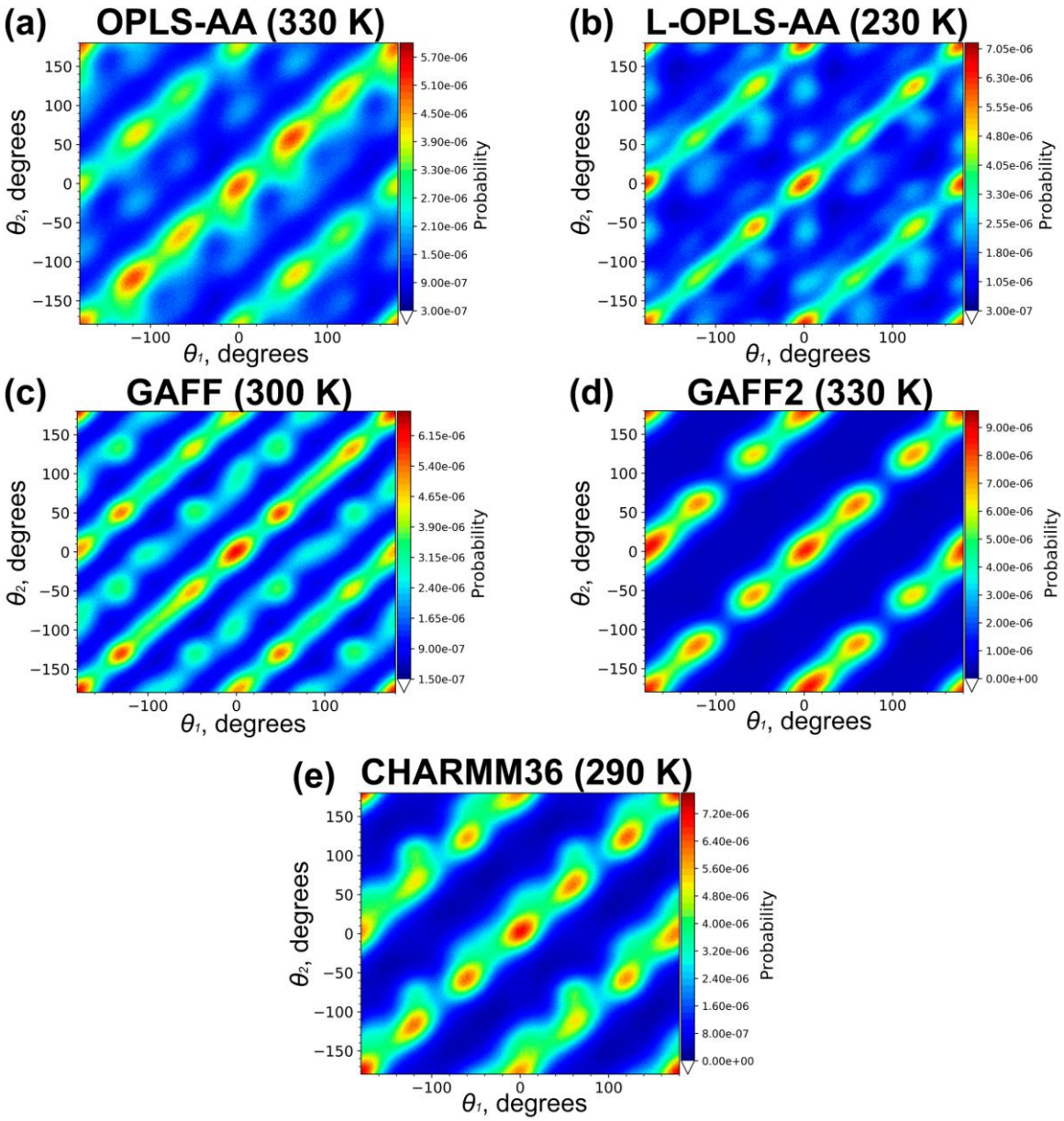

Fig. S9. The probability distribution $P(\theta_1,\theta_2)$ for the n-eicosane crystalline phase simulated with the use of all-atom models at temperatures that are 30-35 K lower than the crystallization temperature. Show are results for configuration 1.

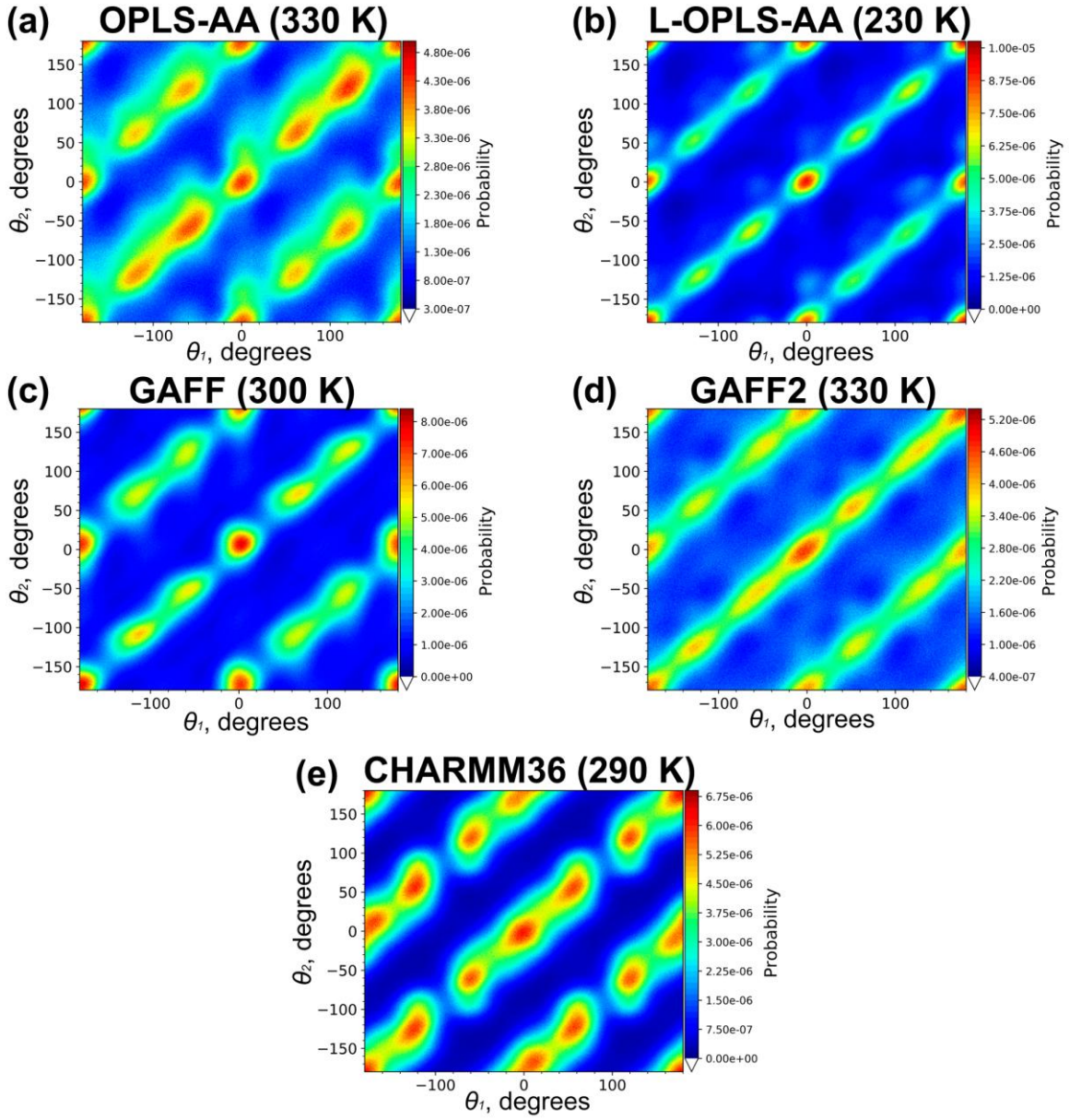

Fig. S10. The probability distribution $P(\theta_1,\theta_2)$ for the n-eicosane crystalline phase simulated with the use of all-atom models at temperatures that are 30-35 K lower than the crystallization temperature. Show are results for configuration 2.

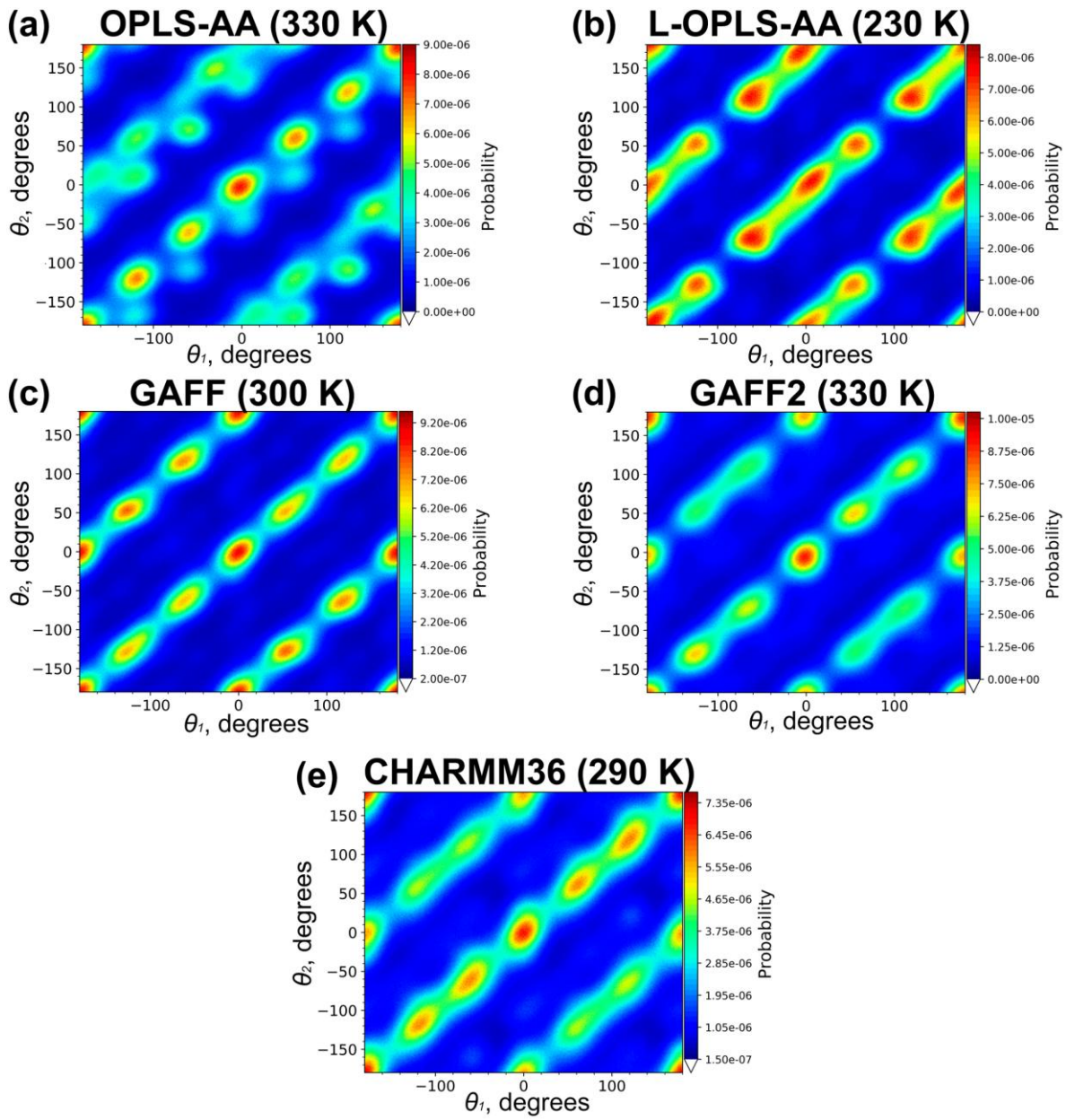

Fig. S11. The probability distribution $P(\theta_1,\theta_2)$ for the n-eicosane crystalline phase simulated with the use of all-atom models at temperatures that are 30-35 K lower than the crystallization temperature. Show are results for configuration 3.

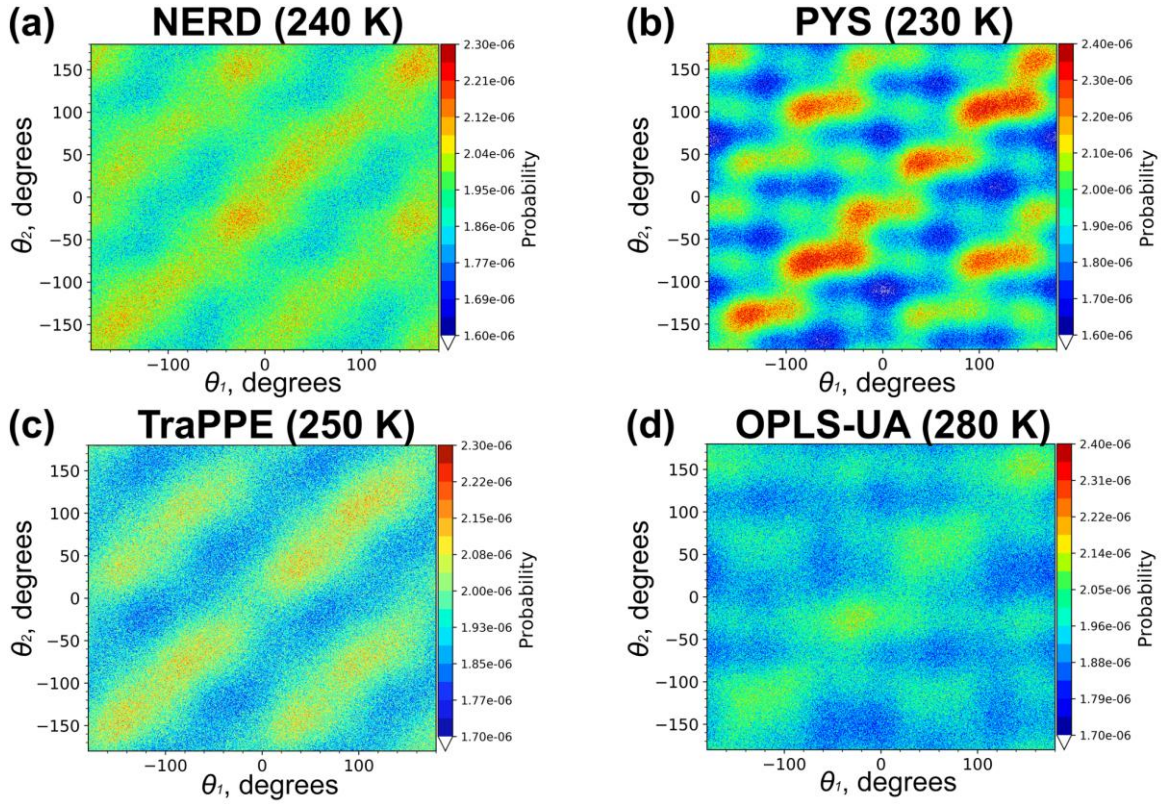

Fig. S12. The probability distribution $P(\theta_1,\theta_2)$ for the n-eicosane crystalline phase simulated with the use of united-atom models at temperatures that are 30-35 K lower than the crystallization temperature. Show are results for configuration 1.

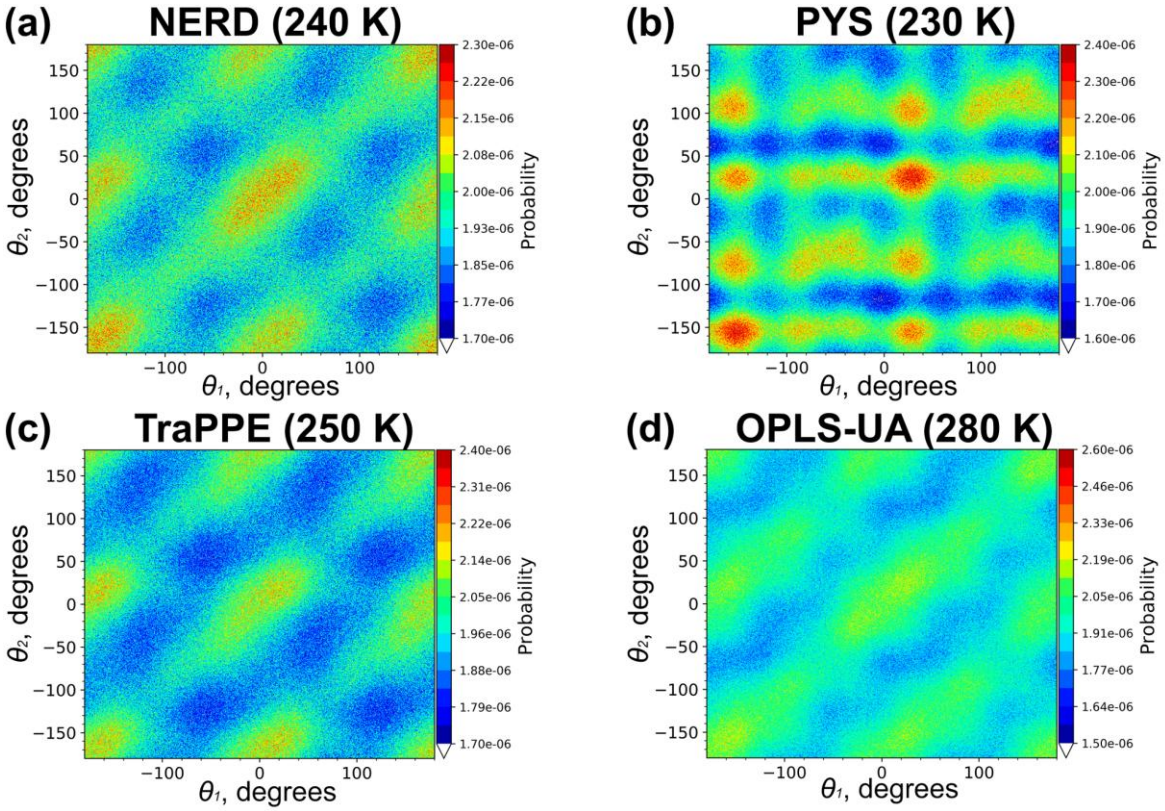

Fig. S13. The probability distribution $P(\theta_1,\theta_2)$ for the n-eicosane crystalline phase simulated with the use of united-atom models at temperatures that are 30-35 K lower than the crystallization temperature. Show are results for configuration 2.

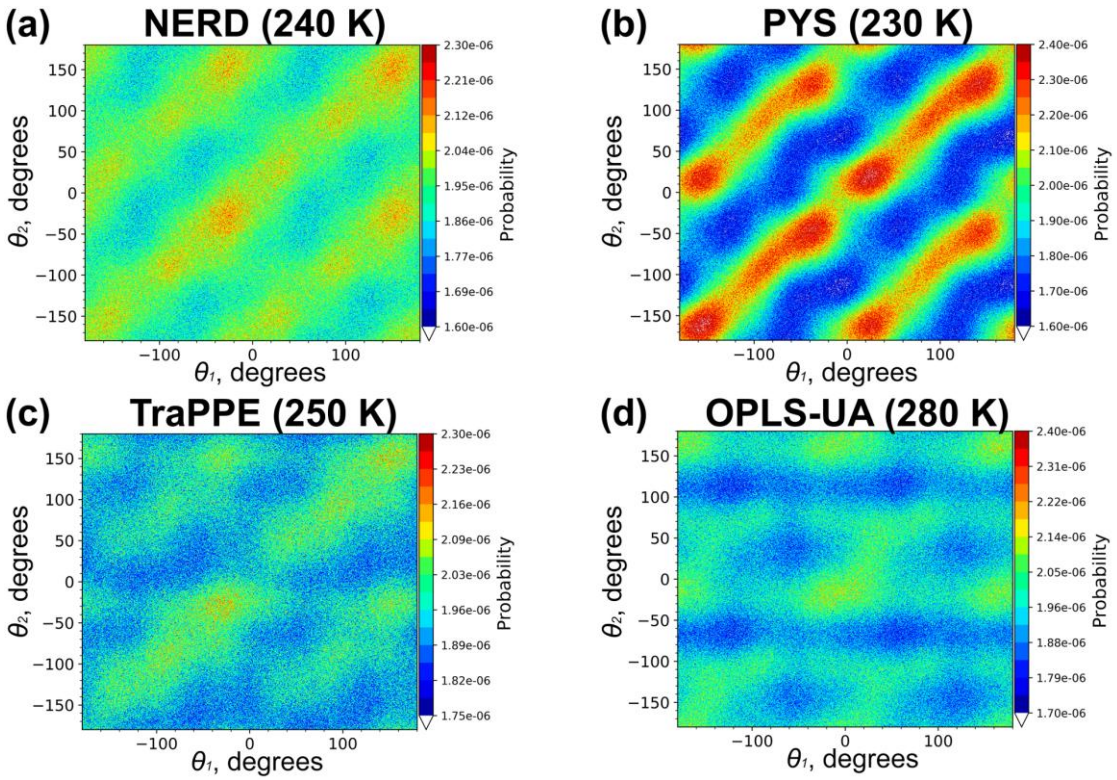

Fig. S14. The probability distribution $P(\theta_1,\theta_2)$ for the n-eicosane crystalline phase simulated with the use of united-atom models at temperatures that are 30-35 K lower than the crystallization temperature. Show are results for configuration 3.

References

1 W.F. Seyer, R.F. Patterson and J.L. Keays, *J. Am. Chem. Soc.*, 1944, **66**, 179-182.