Dansk Fysisk Selskab

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The EXP pair-potential system

It was recently shown that the exponentially repulsive EXP pair potential defines a system of particles in terms of which simple liquids'quasiuniversality may be explained[a,b]. The quasiuniversality was illustrated by showing that the structure of the Lennard-Jones system at four state points is well approximated by those of EXP pair-potential systems with the same reduced diffusion constant[c].

The fluid phase of the EXP pair potential system was studied in two companion papers[c,d]. The study revealed the existence of two regions in the fluid: A gas phase and a liquid phase which are distinguished pragmatically by the absence or presence of a minimum in the radial distribution function above its first maximum. The existence of isomorphs has been found in both the dilute gas phase, and in the condensed liquid. The simplicity of the gas phase allows for predictions of the virial potential-energy Pearson correlation coefficient R and the density-scaling exponent in the dilute limit.
In the latest work[e] also the crystal phase has been studied and both a bcc phase and a fcc phase has been found.

a: Bacher, A. K., Schrøder, T. B. & Dyre, J. C. Explaining why simple liquids are quasi-universal. Nat. Comm. 5, 5424 (2014)
b: Dyre, J. C. Topological review: Simple liquids'quasiuniversality and the hard-sphere paradigm. J. Phys. Condens. Matter 28, 323001 (2016)
c: Bacher, A. K., Schrøder, T. B. & Dyre, J. C. The EXP pair-potential system. I. Fluid phase isotherms, isochores, and quasiuniversality. J. Chem. Phys. 149, 114501 (2018)
d: Bacher, A. K., Schrøder, T. B. & Dyre, J. C. The EXP pair-potential system. II. Fluid phase isomorphs. J. Chem. Phys. 149, 114502 (2018)
e: Pedesen, U. R., Bacher, A. K., Schrøder, T. B. & Dyre, J. C. The EXP pair-potential system. III. Thermodynamic phase diagram. J. Chem. Phys. 150, 174501 (2019)

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