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Abstract book

List of Communications

M1.2 S. Vasiliev, J. Ahokas, J. Järvinen, L. Lehtonen, S. Sheludiakov, V.V. Khmelenko, D.M. Lee, & Yu.A. Dmitriev (Turku, FI; College Station, TX, US; St Petersburg, RU) *Evidence for a solid-to-liquid transition of molecular hydrogen inside pores of solid neon below 1 K.*

M1.3 S. Sheludiakov, P.T. McColgan, D.M. Lee, V.V. Khmelenko, J. Ahokas, J. Järvinen, and S. Vasiliev (College Station, TX, US; Turku, FI) *Formation of a highly nuclear polarized state of H atoms embedded in solid H_2 films.*

M2.6 E. Yakub (Odessa, UA) *The role of short- and long-range forces in formation of orientational structure of simple molecular crystals.*

M3.9 L. Firlej & B. Kuchta (Montpellier & Marseille, FR) *On the non-uniform density of gases confined in nanopores.*

M4.11 I. Iwasa (Kanagawa, JP) *Internal structure of solid ^{4}He observed by X-ray topography.*

M4.12 L. Yakub & E.S.Bodiul (Odessa, UA) *Thermodynamic properties of CH_4, CCl_4 and CF_4 on the melting line. Theory and computer simulation.*

T1.3 B. Kuchta, L. Firlej, F. Formalik, B. Mazur, & Ph. Llevellyn (Marseille & Montpelier, FR; Wrocław, PL) *Adsorption induced low temperature transformations of methane adsorbed in MOF-5.*

T2.6 J. Hasik, E. Tosatti, & R. Martonak (Bratislava, SK; Trieste, IT) *Quantum and classical ripples in graphene.*

T3.9 A. Krivchikov, M. Strzhemechny, A. Jeżowski, & D. Szewczyk (Kharkov, UA; Wrocław, PL) *Low-lying optic modes influence on low temperature heat capacity of molecular crystals.*

T4.11 R.V. Nikonkov, P. Stachowiak, & A. Jeżowski (Wrocław, PL) *Scattering of phonons by palladium and silica nanoparticles embedded in solid nitrogen matrix.*

T4.12 A. Buchachenko, D.S. Bezrukov, & G.K. Ozerov (Moscow, RU) *Computational study of the stable atomic trapping sites in Ar lattice.*

H1.3 V. Efimov, L. Kondaurova, & A. Orlova () *Formation and Decay of Vortex System in Superfluid Helium.*

H2.6 E. Savchenko, I. Khyzhniy, S. Uyutnov, M. Bludov, & V. Bondybey (Kharkov, UA; Garching, DE) *Emission spectroscopy of solid methane.*

H3.9 Yen Fei (Shenzhen, CN) *Magnetic ordering of protons in hexamethylbenzene.*

Thermodynamic Properties of CH_4, CCl_4 and CF_4 on the Melting Line. Theory and Computer Simulation.

L.N. Yakub and **E.S. Bodiul**

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Wide application of methane and its derivatives in low-temperature technology as well as recently discovered presence of condensed methane on surfaces of several celestial bodies make it essential studying their properties in a wide range of temperatures and pressures.

We performed an investigation of the thermodynamic properties of condensed phases of tetrafluoromethane CF_4 and carbon tetrachloride CCl_4 on the melting line and in the high-pressure region using the equation of state developed earlier for methane [1] within the framework of thermodynamic perturbation theory, where octupole-octupole interaction of molecules was treated as perturbation.

We also present the results of Monte Carlo computer simulations of the FCC phases of methane and carbon tetrachloride, as well as the monoclinic phase of tetrafluoromethane using the potential interaction model that takes into account both the central and octupole-octupole interactions [2]. The computer simulation data are compared with available experimental data and results of our calculations based on the equations of state for CH_4, CF_4, and CCl_4.

The contribution of the octupole-octupole interaction to various thermodynamic properties in the solid and liquid phases is estimated. The limits of applicability of the equations of state for solid and liquid phases of methane and its halogen derivatives are discussed.

References

[1] L.N. Yakub and O.S. Bodiul., *J. Low Temp. Phys.* **187**, 33 (2017).
[2] P. Isnard, D. Robert, and L. Galatry. *Mol. Phys.* **31**, 789 (1976).