

Computational search for new Th-H high- T_C superconductors at moderate pressures

A.G. Kvashnin^{1,2}, I.A. Kruglov^{2,3}, D.V. Semenov¹, A.R. Oganov^{1,2,3,4},

¹ Skolkovo Institute of Science and Technology, Skolkovo Innovation Center 121205, 3 Nobel Street, Moscow, Russia

² Moscow Institute of Physics and Technology, 141700, 9 Institutsky lane, Dolgoprudny, Russia

³ Dukhov Research Institute of Automatics (VNIIA), Moscow 127055, Russia

⁴ Northwestern Polytechnical University, Xi'an, 710072, China

Keywords: high pressure, superconductors, USPEX

*e-mail: A.Kvashnin@skoltech.ru

Hydrogen-rich hydrides attract great attention due to recent theoretical [1] and then experimental discovery of record high-temperature superconductivity in H₃S ($T_C = 203$ K at 155 GPa [2]).

Here we perform a systematic evolutionary search for new phases in the Fe-H [3], Th-H [4], U-H [5] and other numerous systems under pressure [6] in order to predict new materials which are unique high-temperature superconductors.

We predict new hydride phases at various pressures using the variable-composition search as implemented in evolutionary algorithm USPEX [7-9]. Among the Fe-H system two potentially high- T_C FeH₅ and FeH₆ phases in the pressure range from 150 to 300 GPa were predicted and were found to be superconducting within Bardeen-Cooper-Schrieffer theory, with T_C values of up to 46 K. Several new thorium hydrides were predicted to be stable under pressure using evolutionary algorithm USPEX, including ThH₃, Th₃H₁₀, ThH₄, ThH₆, ThH₇ and ThH₁₀. Fm $\bar{3}$ mThH₁₀ was found to be the highest-temperature superconductor with T_C in the range

221-305 K at 100 GPa. Actinide hydrides show, i.e. AcH₁₆ was predicted to be stable at 110 GPa with T_C of 241 K.

To continue this theoretical study, we performed an experimental synthesis of Th-H phases at high-pressures including ThH₁₀. Obtained results can be found in Ref. [10].

Acknowledgments: This work was supported by RFBR foundation № 19-03-00100 and facie foundation, grant UMNK №13408GU/2018.

- [1] D. Duan et al., *Sci. Rep.* 2018, **4**, 6968.
- [2] A.P. Drozdov et al. *Nature*. 2015, **525**, 73–76.
- [3] A.G. Kvashnin et al. *J. Phys. Chem. C* 2018, **122** 4731-4736.
- [4] A.G. Kvashnin et al. *ACS Applied Materials & Interfaces* 2018, **10**, 43809–43816.
- [5] I.A. Kruglov et al. *Sci. Adv.* 2018, **4**, eaat9776.
- [6] D.V. Semenov et al. *J. Phys. Chem. Lett.* 2018, **8**, 1920-1926.
- [7] A.O. Lyakhov et al. *Comp. Phys. Comm.* 2013, **184**, 1172-1182.
- [8] A.R. Oganov et al. *J. Chem. Phys.* 2006, **124**, 244704.
- [9] A.R. Oganov et al. *Acc. Chem. Res.* 2011, **44** 227-237.
- [10] D.V. Semenov et al. 2019, arXiv:1902.10206.