Abstract Submitted for the MAR17 Meeting of The American Physical Society

Many-electron effects at extreme conditions.¹ IGOR ABRIKOSOV, Linkping Unversity, Sweden and NUST "MISIS", Russia — Using theoretical simulations at the level of Dynamical Mean-Field Theory combined with DFT (DFT+DMFT) coupled to advanced experimental studies of materials at extreme conditions we show that many-electron effects have strong influence on the electronic structure and properties of transition metals, their alloys and compounds. In particular, correlation effects are essential for a description of the pressure induced insulator-to-metal transitions (IMT). We illustrate this by considering IMTs in transition metal oxides [1,2]. Moreover, considering https://www.ee.and.org/tech.ee.and. that including correlation effects is necessary for the description of the topological changes of the Fermi surface for valence electrons at high pressure, the so-called electronic topological transition (ETT) [3,4]. Considering Fe at the conditions of the Earth's core, we show that DFT+DMFT calculations allow one for better understanding of the Earth's geodynamo [5,6]. [1] V. Potapkin et al., Phys. Rev. B 93, 201110(R) (2016). [2] I. Leonov et al., Phys. Rev. B 94, 155135 (2016). [3] K. Glazyrin, et al., Phys. Rev. Lett. 110, 117206 (2013). [4] L. Dubrovinsky et al., Nature 525, 226–229 (2015). [5] L. V. Pourovskii et al., Phys. Rev. B 87, 115130 (2013). [6] L. V. Pourovskii et al., arXiv:1603.02287 [cond-mat.str-el].

¹The Swedish Research Council (VR) Grant No. 2015-04391 and the Grant of Ministry of Education and Science of the Russian Federation in the framework of Increase Competitiveness Program of NUST MISIS (No. K2- 2016-013) are gratefully acknowledged

> Igor Abrikosov Linkping Unversity

Date submitted: 16 Nov 2016

Electronic form version 1.4