Many-electron effects at extreme conditions. IGOR ABRIKOSOV, Linkping University, 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 hcp Fe and Os, we show 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].


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.