Contribution ID: **1667** Type: **Oral**

Point defects in $FeMe_2O_4$ (Me = Fe, Cr) spinels: a DFT+U investigation in the light of experimental data

Thursday 31 October 2024 16:30 (15 minutes)

Spinel-type crystals AMe_2O_4 encompass a wide range of practical applications like photocatalysis or spintronics, but often demonstrate non-trivial electronic and magnetic properties which theoretical description is mitigated. In this work, we performed DFT+U calculations for the most extensive set of neutral point defects in Fe_3O_4 (magnetite) and $FeCr_2O_4$ (chromite) and investigated all the possible types of cationic and oxygen defects in both spinels. Our results unveil both similarities and principal differences between the defective Fe_3O_4 and $FeCr_2O_4$, posing chromite as a material less prone to defect formation, and could be a valuable asset to the development of new multiscale models of steel corrosion. For more details, readers are referred to [JETP, 166(3), 347, 2024].

Primary authors: CHICHEVATOV, Gleb (Joint Institute for High Temperatures RAS, Moscow Institute of Physics and Technology); STEGAILOV, Vladimir (JIHT RAS)

Presenter: CHICHEVATOV, Gleb (Joint Institute for High Temperatures RAS, Moscow Institute of Physics and Technology)

Session Classification: Condensed Matter Physics

Track Classification: Condensed Matter Physics