Secteur des Sciences et Technologies

Invitation à la soutenance publique de thèse de
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Pour l'obtention du grade de Docteur en sciences de l'ingénieur et technologie

« Insights into the physical properties of the MAX phases and MXenes: From experiments to first-principles modeling »

qui se déroulera
le jeudi 03 septembre 2020 à 15h
Auditoire A01 SCES
Place des Sciences
1348 Louvain-la-Neuve

Jury members :

Prof. Jean-Christophe Charlier (UCLouvain), supervisor
Prof. Bernard Nysten (UCLouvain), chairperson
Prof. Gian-Marco Rignanese (UCLouvain), secretary
Prof. Benoît Hackens (UCLouvain)
Prof. Michel W. Barsoum (Drexel University, USA)
Prof. Thierry Ouisse (Univ. Grenoble-Alpes, France)
Prof. Matthieu J. Verstraete (ULiège, Belgium)

The MAX phases are nanolayered transition metal carbides and nitrides characterized by a unique combination of metal and ceramic-like properties, which makes them good candidates in electrical contacts, micro-mechanical systems, and high-temperature applications. The recent addition of new MAX compositions and atomic ordering brings the total amount of existing MAX phases to 155, most of which still await both experimental characterization and theoretical investigation of their properties. In this thesis, the growth of high-quality single-crystals of ternary Cr_2AlC and quaternary RE-i-MAX phases is presented. An experimental study of their vibrational and elastic properties is performed. Additionally, the structural, electronic, vibrational, thermal, and elastic properties of these 3D compounds are calculated from first principles. While the elastic properties of the MAX phases are isotropic, a noticeable anisotropy in their electrical, vibrational, and thermal properties is predicted theoretically and, in some cases, verified experimentally. Finally, a complete analysis of the bonding strengths and exfoliation energies is performed, predicting the potential exfoliation of these 3D systems into 2D ones. In 2011, the MAX phases were successfully exfoliated into 2D systems, called MXenes. They draw interest due to their unique properties combining high electrical conductivity, large surface area, and hydrophilicity. In this thesis, the structural, electronic, and vibrational properties of the V_2CT_z MXene are computed ab initio. In parallel, experiments are conducted to synthesize the 2D V_2CT_z MXene from its parent V_2AlC MAX phase and to characterize its Raman response. The phonon mode wavenumbers, symmetries, activities, and associated atomic displacements are investigated.