Contribution ID: **34** Type: **Poster**

Density Functional Theory study of Cd impurities in Molybdenum Trioxide

Wednesday 15 December 2021 17:23 (3 minutes)

Transition metal oxides semiconductors (TMOs) are known for their special optical and electrical properties with wide-ranging applications, including gas sensing, storage devices such as Li-ion batteries, solar cells, and catalysts[1,2]. Among different types of TMOs, there is a class of materials that are distinguished by their unique layered structure and multiple oxidation states, such as MoO_3, WO_3, and V_2O_5. The molybdenum trioxide (MoO_3) is known for its photo-, thermo- and electro-chromism, high catalytic activity[3]. The MoO_3 has found in different structural phases including the orthorhombic phase, α-MoO_3; monoclinic phase, β-MoO_3; metastable phase at high-pressure conditions, β′-MoO_3; and hexagonal phase, h-MoO_3[4]. Among them, the α-MoO_3 is the most stable crystal phase and it has a layered structure consisting of van der Waals bonded sheets of distorted edge-sharing Mo–O_6 octahedra in which Mo atoms are bounded by three distinct types of oxygen atoms[5].

In this research, the structural properties and hyperfine parameters of ^{111m}Cd(^{111}Cd) impurities in α-MoO_3 are investigated by first-principle calculations in the framework of density functional theory (DFT). The Perdew–Burke–Ernzerh of generalized gradient approximation (GGA-PBE), and GGA-PBE plus Hubbard-U corrections for onsite Coulomb interactions are used in the DFT calculations. In the calculations performed, the effect of van der Waals forces between layers is employed using the DFT-D3 method[6]. To interpret the experimental results, different configurations around the Cd atom including the different types of oxygen vacancies are simulated. The comparison of experimental data with calculated hyperfine parameters indicates that the Cd atom is predominantly located in the interstitial lattice site of MoO_3, and also the oxygen vacancy is most likely to form on the 2-fold coordinated (O_2) atoms.

The results of this work demonstrate the benefit of first-principle calculations for solving the outstanding questions arising from the experiment.

References:

1. Kalantar-zadeh, Kourosh, et al. , Applied Materials Today 5 (2016): 73-89.
2. Hu, Guangwei, et al., Nature 582.7811 (2020): 209-213.
3. Fleisch, T. H., and G. J. Mains., The Journal of chemical physics 76.2 (1982): 780-786.
4. Wang, Lu, et al. , High Temperature Materials and Processes 39.1 (2020): 620-626.
5. Peelaers, H., M. L. Chabinyc, and C. G. Van de Walle., Chemistry of Materials 29.6 (2017): 2563-2567.
6. Grimme, Stefan, et al., The Journal of chemical physics 132.15 (2010): 154104.

Author: MOKHLES GERAMI, Adeleh (Institute for Research in Fundamental Sciences (IR))

Co-authors: SCHELL, Juliana (Institut Fur Materialwissenschaft Universität Duisburg-Essen (DE)); CARBONARI, Artur (IPEN); SANTOS COSTA, Messias (Faculdade de Ciencias Exatas e Tecnologia, Universidade Federal do Pará, 68440-000 Abaetetuba, PA, Brazil); COSTA, Cleidilane (Faculdade de Ciencias Exatas e Tecnologia, Universidade Federal do Pará, 68440-000 Abaetetuba, PA, Brazil); DIAZ-GUERRA VIEJO, Carlos (Departamento de Física de Materiales, Facultad de Ciencias Físicas, Universidad Complutense de Madrid, Ciudad Universitaria s/n, 28040 Madrid, Spain); LORENZ, Katharina (Universidade de Lisboa (PT)); PIRES, Julio (Universidade de Lisboa (PT)); MONTEIRO, Joao (Universidade de Lisboa (PT)); JOHNSTON, Karl (CERN); MARTINS CORREIA, Joao (Universidade de Lisboa (PT))

Presenter: MOKHLES GERAMI, Adeleh (Institute for Research in Fundamental Sciences (IR))

Session Classification: Poster Presentations