Presentation title: Enhancing magnetic properties and Curie temperature of 4d and 5d transition metal and p-block element co-doped Fe_2P alloys

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Enhancing magnetic properties and Curie temperature of 4d and 5d transition metal and p-block element co-doped Fe_2P alloys

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Abstract:

Permanent magnets are ubiquitous in modern technology, playing a vital role in countless applications that permeate our daily lives. These unassuming yet powerful materials have found their way into an array of devices, from electric motors to medical equipment, and are pivotal in emerging technologies like renewable energy generation and electric vehicles. Among the various materials used for permanent magnets, standout contenders are Fe_2P alloys. Iron phosphide (Fe_2P) alloys exhibit excellent magnetic properties and could be used as a candidate to fill the gap magnets between hard ferrite and rare-earth based permanent magnet (PM) applications. However, one of the major problems with Fe_2P is the low Curie temperature (T_c) compared with other PM materials. The electronic structure, magnetic properties, exchange interaction (J_{ij}) and Curie temperature (T_c) of $M_{0.04}Fe_{2-x}P_{y-1}Z_y$ (M = 4d and 5d heavy transition metals, and Z = p-block elements such as B, C, N for 2ndrow, Al, Si and S for 3rdrow and Ga, Ge, As and Se for 4throw) alloys are investigated using the first-principles method, within the framework of density functional theory (DFT). Our result indicate that the value of magneto-crystalline anisotropy constant on the Os doping element for the 5d transition metals is enhanced up to 3.32 MJ/m^3, which is higher than that for the pristine Fe_2P alloy due to the

spin-orbit coupling of high nuclear charge and close to the half-filled electron configurations. It is 10% higher than for pristine Fe_2P making it suitable for PM applications. We show that the Curie temperature (T_c), magnetic saturation (M_s) and energy product (BH_{max}) is increasing on the $M_{0.04}Fe_{2-x}P_{y-1}Z_y$ (M = Ru, Os, Pt heavy transition metals, and Z = B group (B, Al, Ga) elements). This suggests the potential for these materials as viable candidates for permanent magnet applications.
In addition, preliminary results of our density-functional theory calculations through the collaborations with our collaborators at the Incheon National University, South Korea, and Oak Ridge National Laboratory, USA, for the specified alloys, will be presented.

Biography:

Khongorzul Baatartsogt is a dedicated physicist and Ph.D. student specializing in material science, with a notable expertise in density functional theory (DFT). Since 2016, Khongorzul has been a researcher of the Mongolian Academy of Sciences, Institute of Physics and Technology, where their research efforts have significantly advanced our understanding of materials and their properties.

With a solid foundation in physics from the National University of Mongolia, Khongorzul Baatartsogt has made substantial contributions to the field of material science through their extensive publications in Web of Science (WOS) journals. Their utilization of density functional theory in these publications has provided valuable insights into the atomic and electronic structures of various materials, paving the way for applications.

Recognized for their scholarly achievements, Khongorzul Baatartsogt is regarded as a promising young scholar in the scientific community. Their commitment to excellence and passion for scientific inquiry continue to drive their research endeavors, positioning them as a key contributor to the advancement of physics and material science.

Excited about the opportunity to engage with fellow researchers, Khongorzul Baatartsogt looks forward to participating in the upcoming conference, where they aim to share their expertise, foster collaborations, and further contribute to the collective knowledge in their field.