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Exploring High Entropy Alloys for Next-Generation Beam Windows: A Computational Approach

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Beam power and runtime in high energy particle accelerators are currently limited by targets and beam windows. The existing materials used in these components have reached their maximum potential, necessitating the development of a new class of materials known as high entropy alloys (HEAs) to overcome this challenge. Numerous studies have demonstrated that HEAs possess exceptional qualities such as high strength, ductility, and radiation resistance. In this study, we propose an approach that utilizes computational techniques including CALPHAD, density functional theory (DFT), and molecular dynamics (MD) to investigate and comprehend the defect properties of suitable HEAs, which can serve as alternative materials for the next generation of beam windows. Initially, CALPHAD is employed to conduct approximately one hundred thousand simulations, enabling us to narrow down the potential compositions to a select few. Subsequently, we intend to employ a DFT-informed machine learning potential to analyze the defect properties of these narrowed compositions. During this presentation, I will outline the CALPHAD approach implemented to refine the compositions, elucidate the necessity of DFT, and demonstrate the potential usefulness of machine learning in this context.

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