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Machine Learning-Assisted Design of Cesium-Based Photocathodes from First Principles

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Cesium-based photocathodes, such as cesium-telluride, are commonly used as electron sources in particle accelerators. Yet, precise control over these materials is hindered by challenges in regulating their crystal structure and stoichiometry during synthesis. While ab initio methods such as density functional theory (DFT) can successfully complement experimental efforts, they also require structural information as an input. Hence, the lack of reliable experimental data in this regard limits the potential of computational research and thus their contribution to unveil the fundamental properties of the photocathode materials. To overcome these limitations, we propose a novel approach combining high-throughput DFT calculations with machine learning. Our method predicts stable crystal structures within binary and ternary systems by systematically evaluating various structural descriptors and machine learning algorithms. We demonstrate the superiority of models based on atomic coordination environments, with transfer-learned graph neural networks emerging as a particularly promising technique. By validating our approach on well-characterized Cs-Te materials, we showcase its potential to enhance traditional computational methods and accelerate the development of advanced photocathode materials.

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