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Machine Learning for Materials Discovery[1] BRAYDEN BEKKER, CHANDRAMOULI NYSHADHAM, GUS HART, Brigham Young Univ - Provo, BRIGHAM YOUNG UNIV - PROVO COLLABORATION — Advances in fields from engineering to medicine demand the accurate prediction of new materials at an increased rate. The innumerable combination of materials and high computational cost of accurate predictions limits the ability to produce results at the necessary levels. The recently proposed Many Body Tensor Representation (MBTR)(Huo, Haoyan, and Matthias Rupp. "Unified Representation for Machine Learning of Molecules and Crystals." arXiv preprint arXiv:1704.06439 (2017).) interpolates the materials space to achieve accurate results at a fraction of the computational cost. In this talk, we present the application of MBTR for representing binary/ternary alloys and using machine learning to predict new materials at a faster rate. We show the ability of the MBTR method to meet the increasing demands for fast and accurate materials prediction.

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