

Abstract: NeSA202100poster-05: AFLOW π : Calculations of the Elastic Constants

Time: 12:00-1:00 PM

Presenter:

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The elastic properties of a materials may contain information associated with local distortion and provide the description of mechanical properties of the materials. Using *AFLOW π* , we have implemented and tested the accuracy of the Lagrangian methodology of elastic constants for selected alkali halides with NaCl and CsCl structure. We will discuss our implementation of ElaStic Tool in *AFLOW π* , and the results of elastic constants for selected systems of materials. Our implementation can be used to accelerate materials discovery and design in the technologically important class of materials.