Abstract Submitted
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Integrative interactive visualization of crystal structure, band structure, and Brillouin zone[1] ROBERT HANSON, BEN HINKE, MATTHEW VAN KOEVERING, Saint Olaf College, COREY OSES, CORMAC TOHER, DAVID HICKS, ERIC GOSSETT, JOSE PLATA RAMOS, STEFANO CURTAROLO, Duke University, AFLOW COLLABORATION — The AFLOW library is an open-access database for high throughput ab-initio calculations that serves as a resource for the dissemination of computational results in the area of materials science. Our project aims to create an interactive web-based visualization of any structure in the AFLOW database that has associate band structure data in a way that allows novel simultaneous exploration of the crystal structure, band structure, and Brillouin zone. Interactivity is obtained using two synchronized JSmol implementations, one for the crystal structure and one for the Brillouin zone, along with a D3-based band-structure diagram produced on the fly from data obtained from the AFLOW database. The current website portal (http://aflowlib.mems.duke.edu/users/jmolers/matt/website) allows interactive access and visualization of crystal structure, Brillouin zone and band structure for more than 55,000 inorganic crystal structures.

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