Read Me

File Format

The data for each of the calculated compounds are stored in a list and are provided as a JSON file. For each compound, there are key values, such as "e_electronic" and "e_ionic", that point to the appropriate property (table 1). The key "meta" contains all the appropriate metadata and has its own keys which are one level down in hierarchy. The metadata keys are presented in table 2.

Table 1: Description of keys in the JSON file.

Key	Datatype	Description
e_electronic	array	ϵ_{ij}^{∞} - Dielectric tensor (electronic contribution)
e_total	array	ϵ_{ij} - Total dielectric tensor
poly_electronic	number	ϵ_{poly}^{∞} - Polycrystalline dielectric constant estimate (electronic contribution)
poly_total	number	ϵ_{poly} - Polycrystalline dielectric constant estimate (total)
n	boolean	n - refractive index
band_gap	number	Band gap in the Materials Project database
pot_ferroelectric	boolean	if "True" it signifies a potentially ferroelectric compound
meta	various	metadata - contains details about the structure and DFPT calculation

Table 2: Description of metadata keys

Key	Datatype	Description
material_id	string	Materials Project ID number
formula	string	Chemical formula
structure	string	Crystal structure in Crystallographic Informaiton File (CIF) format
high_forces	boolean	"True" if remnant interatomic forces are larger than 0.01 $eV/$Å
poscar	string	Crystal structure in the VASP-specific poscar format
kpoints	string	k-points in the VASP-specific kpoints format
incar	string	simulation parameters definition file in the VASP-specific incar format
potcar	string	names of the VASP pseudopotentials used for each element
point_group	string	Point group in Hermann-Mauguin notation
space_group	number	Space group number as defined by the International Union of Crystallography
nsites	number	number of atoms in the primitive cell
kpoint_density	number	Number of k-points in the first Brillouin zone per reciprocal atom