Generation of empirical potential parameters for Y and Al doped $BaZrO_3$ systems from *ab initio* data

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Fuel cells are novel means of energy generation featuring a direct means of converting fuels into electricity without going through the combustion progress. Their efficiency is therefore increasingly attracting more interest. Ceramic materials such as perovkites have exhibited great potential as the proton conduction material in one particular kind of fuel cell, the SOFC, or solid oxide fuel cell.

$BaZrO_3$ with two kinds of dopants were investigated: yttrium doped $BaZrO_3$ and aluminum doped $BaZrO_3$. Previous studies in our group have covered their distortion and likely energy pathway in bulk system[12]. However, all these discoveries were based on *ab initio* data from density functional theory calculations of the package VASP, of bulk structures and self-replicating units of smaller size. This limitation in system size, at less than ~500 atoms, proved to be a bottleneck in our investigation of more realistic structures such as grain boundaries, which sometimes would require four digit size supercell to present features such as required dopant density and space charge layers. A computational method that preserves relative accuracy but is capable of handling systems of larger sizes, seems to be of necessity to further our studies on the structure and nature of grain boundary systems.

Buckingham short range potential and coulombic forces long range interaction(using ewald's sum), were used to simulate our system, with the possible addition of partial charges from Mullinken partitioning of DFT. With the help of GULP, the general utility lattice program, and Bader analysis, as well as data from previous group members using DFT and PBE correlational functionals, a set of parameters were extracted to reproduce reasonable lattice size and energy.

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[2] M.A. Gomez, F.-J. Liu, Solid State Ionics (2013), http://dx.doi.org/10.1016/j.ssi.2013.05.014