THEORY AND SIMULATION OF ULTRA-HIGH-TEMPERATURE CERAMICS

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At Imperial College our group contributes theory and simulation advances to the *Materials for Extreme Environments* (XMat) project. Our research supports experiment and industry by developing and applying new high-temperature modelling techniques. These techniques are broad-ranging, from CALPHAD and DFT, to interatomic potentials and analytic models. Here we present advances on each approach and re-cover highlights including:

- the release of MEAMfit, the interatomic potential fitting code
- the development of the TU-TILD approach, for fast and full-order anharmonic thermodynamics [1]
- a new *first-principles*-assisted CALPHAD assessment of ZrC
- analytic models of strain and anharmonicity in carbides and borides
- *ab initio* prediction of intrinsic defects at ultra-high temperatures
- *first principles* heat and charge transport predictions for carbides

Further, we summarise ongoing developments from the theory and simulation group, such as on *first principles* MAX phase thermodynamics.

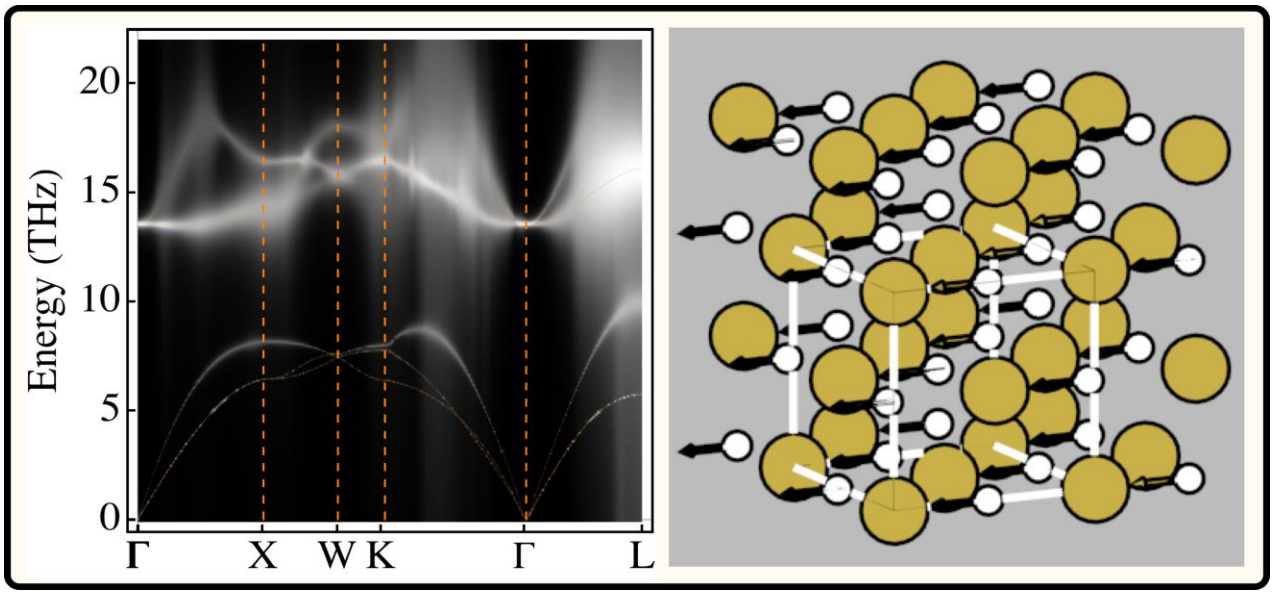

Figure 1 – Phonons in ZrC.

[1] A.I. Duff et al., Physical Review B, 91, 214311, 2015