Evolving a Lattice Dynamics Community:
The role of General Utility Lattice Program (GULP)

Julian D. Gale
Nanochemistry Research Institute, Department of Chemistry, Curtin University, PO Box U1987, Perth, WA 6845, Australia

In this spirit of this symposium, the aim of the present talk will be to provide a perspective on the development of a community focused on the use of force field methods to study problems in the solid-state, and the part played by the GULP program in recent times. In the UK, a large community exists in the area of defect chemistry that nucleated from the proposal of the Mott-Littleton method [1] and rapidly grew with the advent of computer codes, such as HADES from Michael Norgett, which in turn spawned a later generation of codes including PLUTO, CASCADE and MIDAS to name but a few [2]. A key feature of this community was, and remains, the focus on lattice dynamics to compute properties, through the use of analytical higher order derivatives, in contrast to numerical approaches such as molecular dynamics. This is exemplified by the development of free energy minimization techniques based on the quasi-harmonic approximation [3-6]. With an already thriving community, GULP was developed to try to simplify the process of force field development [7] and to improve the efficiency of calculations through the use of symmetry [8]. As the latest version of the program is about to be released, an overview of some of the recent developments, such as addition of reactive force fields [9] and continuum solvation models [10], will be given.

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