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**A Real-Space Genetic Algorithm for Crystal Structure Determination** LUKE ABRAHAM, MATT PROBERT, University of York — There has been much interest in using genetic algorithms for determining the ground-state structure of clusters [1] and nanowires [2], and more recently silicon surfaces [3]. We present a real-space encoded genetic algorithm which is suitable not only for surface structure calculations, but also for bulk crystal structure determination. This algorithm makes use of a novel crossover technique in the generation of offspring. The method is also suitable as a polymorph search, and is flexible enough that population members can have different supercells. We will present results from a variety of empirical and *ab initio* systems, where all calculations have been performed using the CASTEP [4] code.

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