Efficient Internal Coordinate Method for Optimization of Periodic St

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We present a new algorithm for optimizing the structures of periodic systems using delocalized internal coordinates. The method builds on recent concepts developed for molecular optimization due to Pulay, Baker and others. The high coordination of atoms in periodic systems leads to massive numbers of internal coordinates for materials such as close packed metals. Special approaches are introduced for handling the high connectivity of typical solid−state systems.

We shall discuss a number important extensions of the internal coordinate optimization methods. Firstly, we develop an approach for combining internal coordinate optimization with Cartesian constraints, which can be extremely useful for example for studies of surfaces. Secondly we show that by adding carefully selected extra coordinates to the optimization space, it is possible to perform internal coordinate optimization systems where the internal coordinates do not span the optimization space. Typically internal coordinates will fail to span the space when there are disconnected fragments in the unit cell and this second development is particularly important in the treatment of systems such as molecular crystals.

A series of application examples of our method are presented on polymers, molecular crystals, zeolites and semiconductor and catalyst surfaces. It is demonstrated that optimization with internal coordinates for solid−state systems can be much more efficient than the usual methods based on Cartesian coordinates.