Electronic supplementary information for:

Atomic scale modelling of the cores of dislocations in complex materials 2: applications

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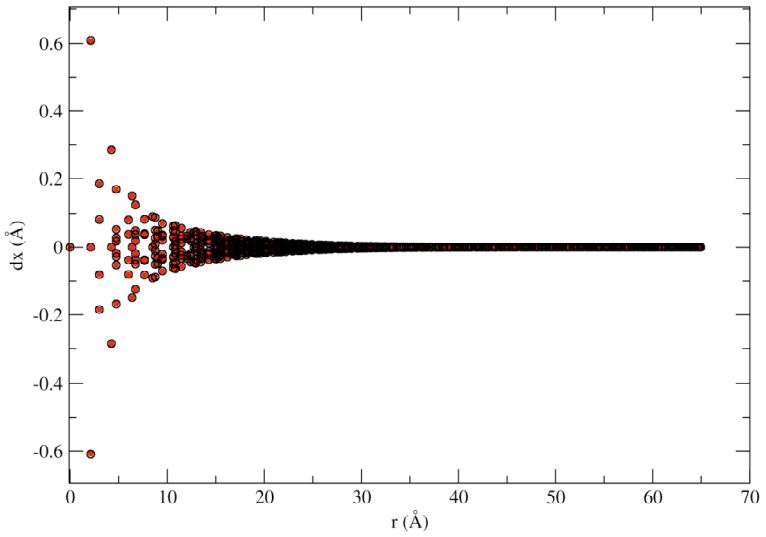
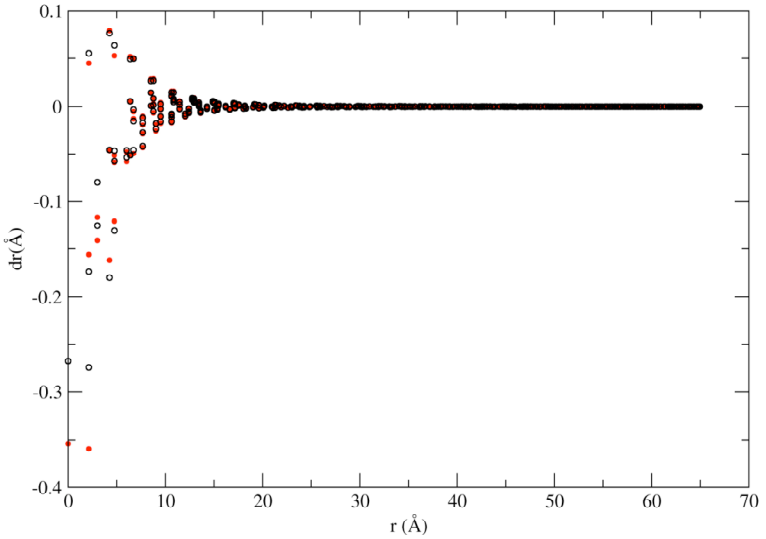
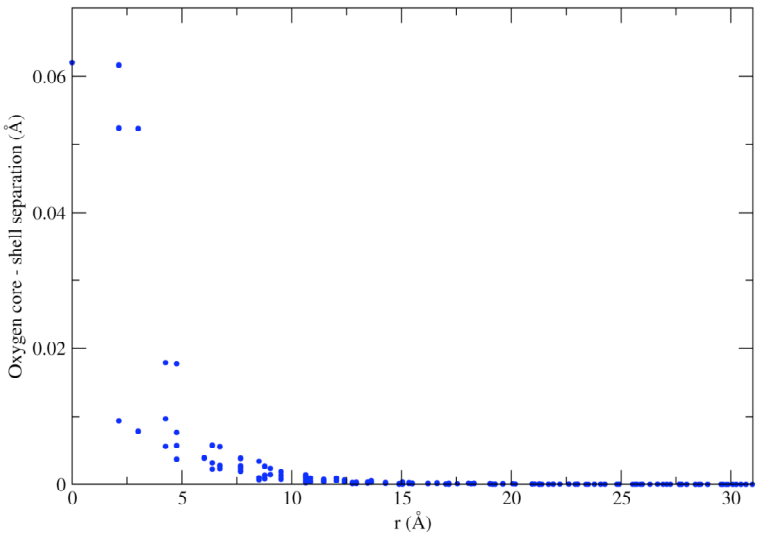


(a)



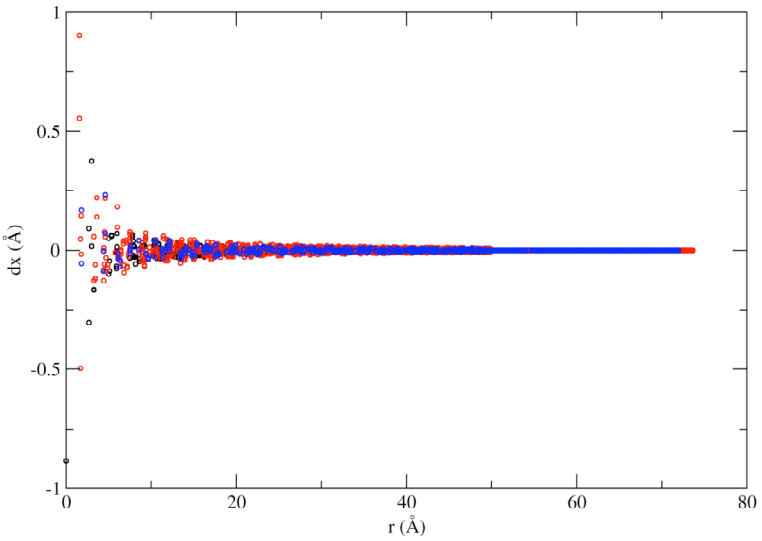
(b)

Figure S1 is continued over the page.

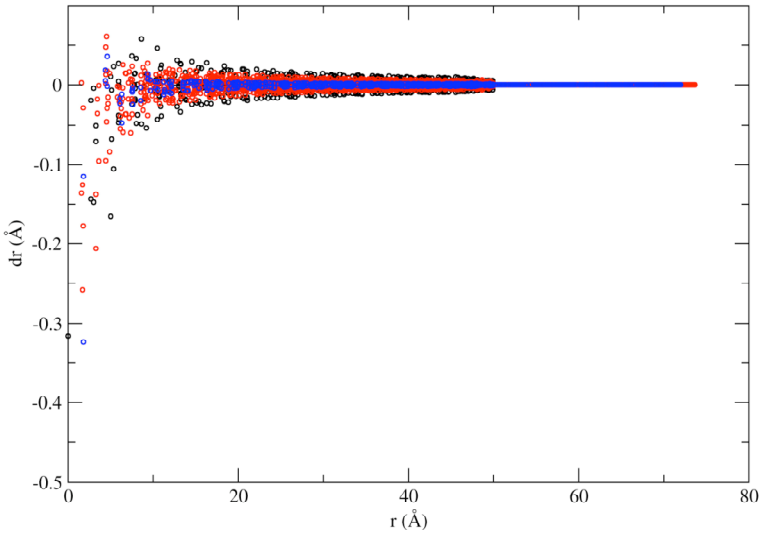


(c)

Figure S1: Relaxation from elastic to atomistic solution for the <100> screw dislocation in MgO (centre site). (a) Ionic displacements parallel to the dislocation line smooth out the discontinuity at the origin. (b) Ionic displacements inwards towards the dislocation line shorten the bond lengths. (c) Oxygen polarisation is rapidly screened out. (Filled red circles: displacement of magnesium ions, open black circles: displacement of oxygen cores, blue filled circles: separation between core and shell centre of breathing shell model.)

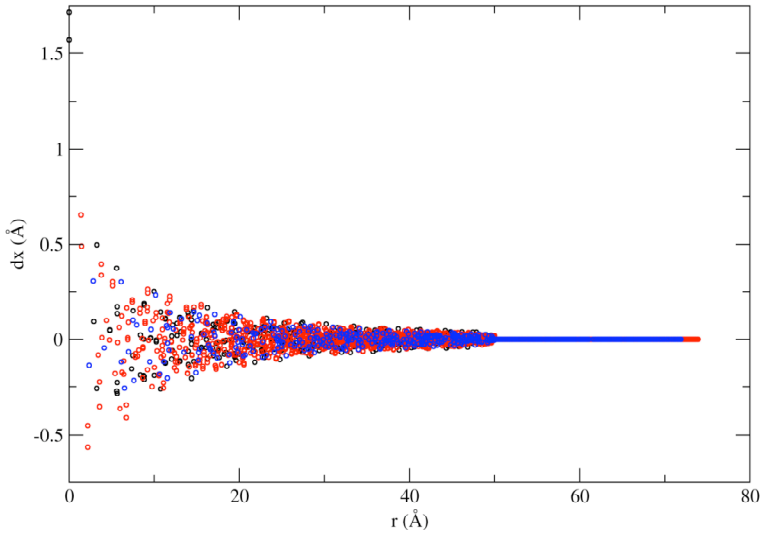


(a)

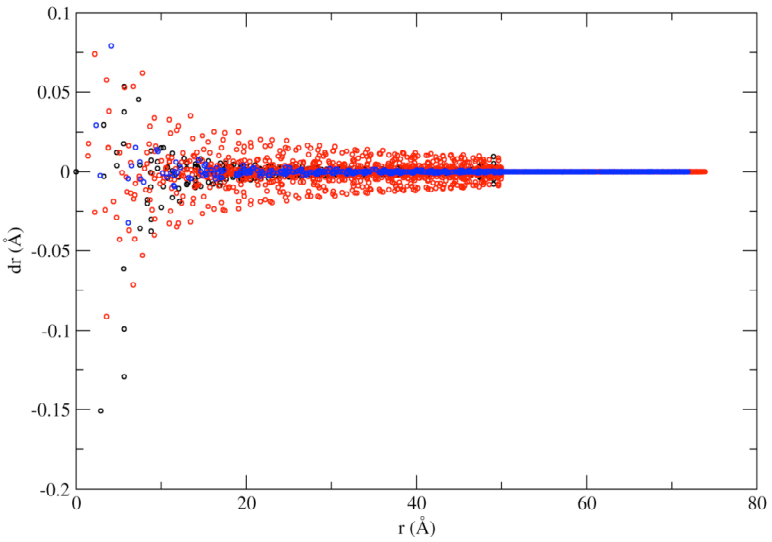


(b)

Figure S2: Relaxation of the atomistic model after introduction of the **a**[100] screw dislocation, movement along the dislocation line is shown in part (a) while movement perpendicular to the dislocation is shown in part (b). Note the large displacement of a magnesium ion along [100] at r=0 shown in part (a). The displacements of silicon ions are shown by blue circles, magnesium ions by black circles and oxygen ions by red circles.

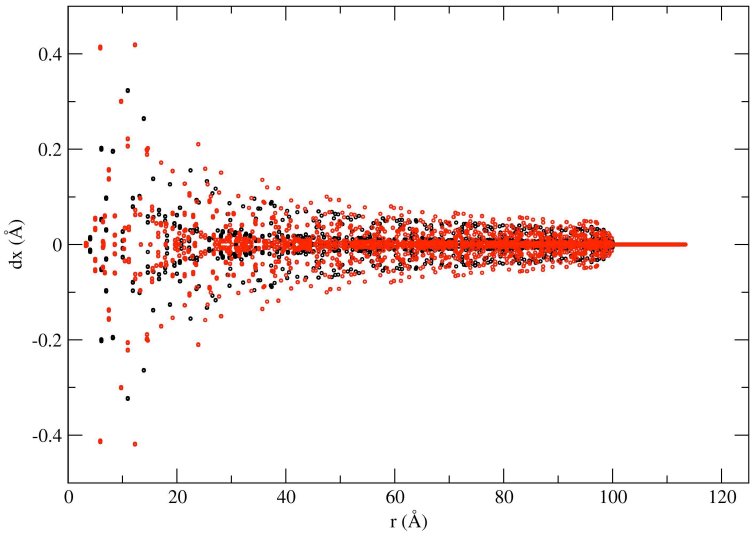


(a)

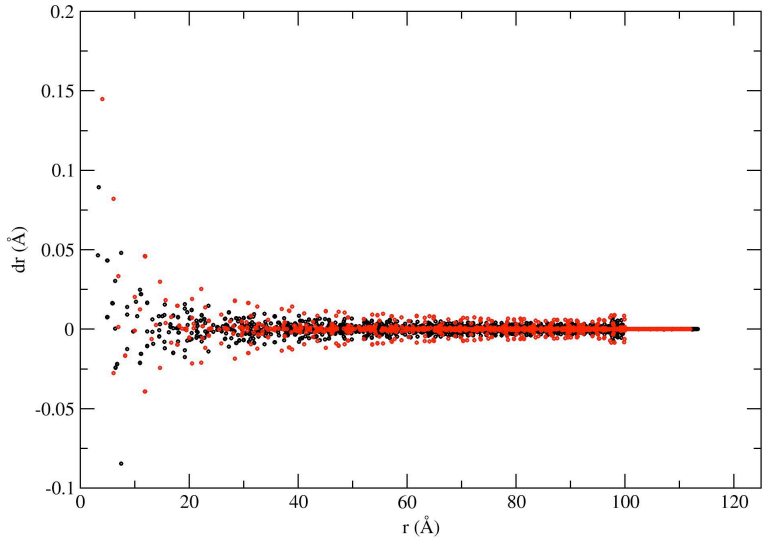


(b)

Figure S3: Core displacement field associated with the **c**[001] screw dislocation in forsterite. Part (a) shows displacements parallel to the dislocation line while part (b) shows displacements perpendicular to the dislocation line. The displacements of silicon ions are shown by blue circles, magnesium ions by black circles and oxygen ions by red circles.



(a)



(b)

Figure S4: Core displacement field associated with 1/2**a** <100> a screw dislocation in siliceous zeolite A. The displacements of oxygen ions are shown in red and the displacements of silicon ions are shown in black. Reproduced from the supplementary information to ref. 20 with permission.

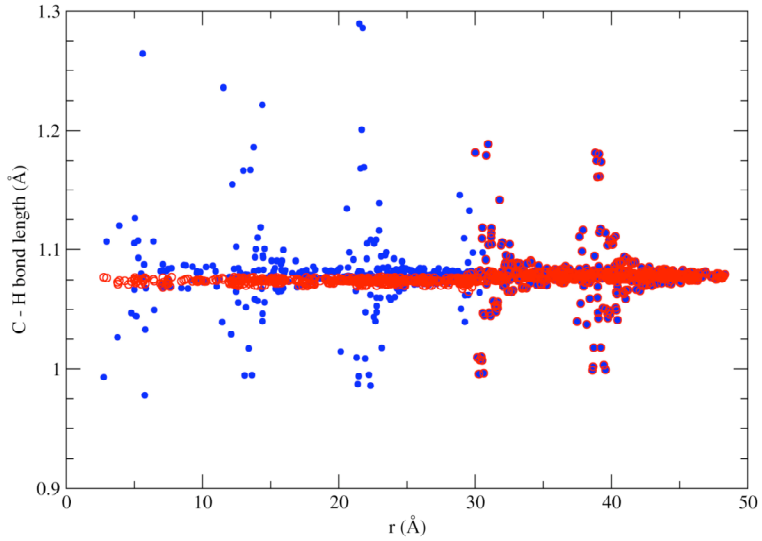
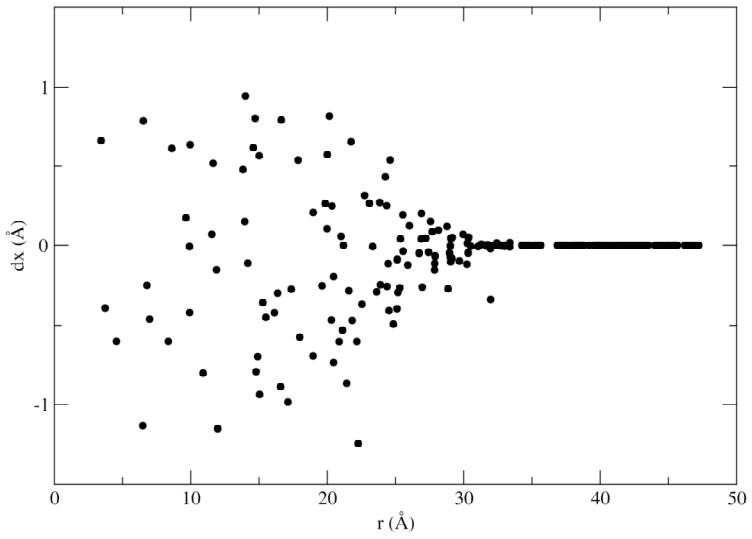
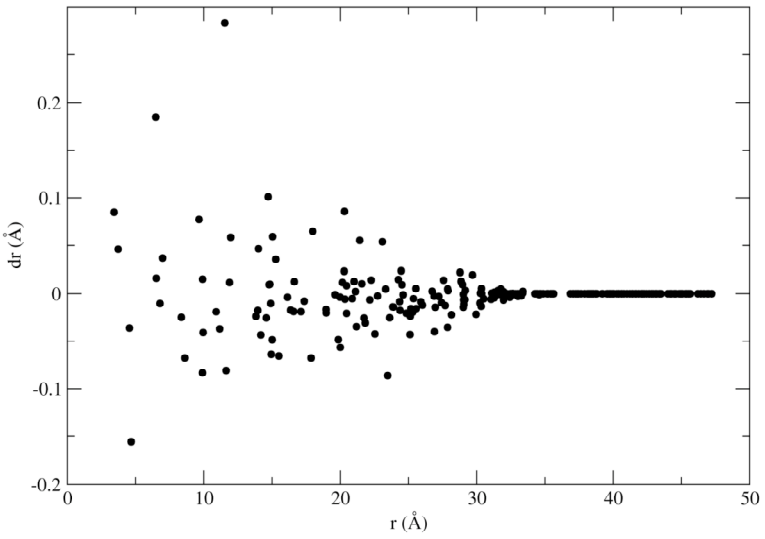


Figure S5: C-H bond lengths around dislocated paracetamol before and after atomic relaxation of the core. Blue circles show the bond lengths after introduction of the dislocation assuming the crystal is a homogeneous linear elastic solid, red open circles show the bond lengths after atomistic relaxation of all atoms within 30 Å of the core to an energy minimum.



(a)



(b)

Figure S6: Core displacement field for the dislocation in paracetamol calculated at the average position of each molecule in the simulation. Part (a) shows molecular displacements along the dislocation line while part (b) shows radial displacements.