Supplementary Material

Atomistic Simulation Study of Diamond Doping Based on Machine Learning Potential

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Convergence test

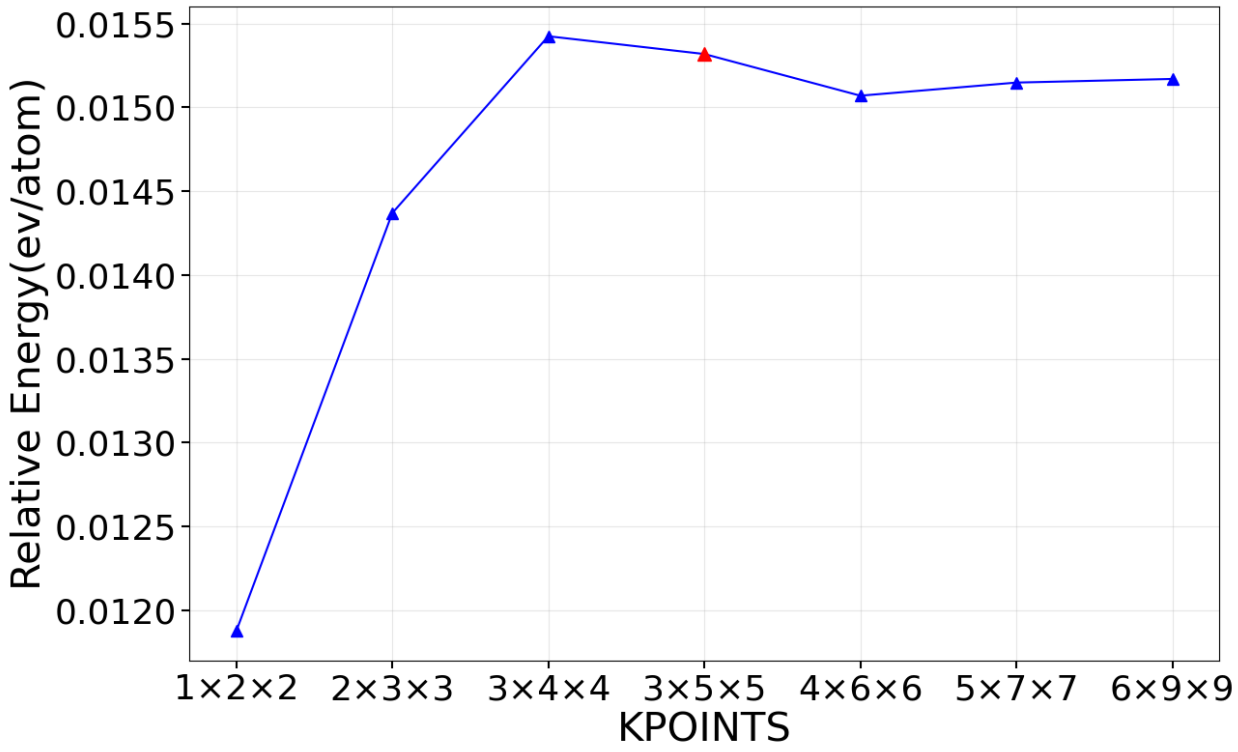

Figure S1: Convergence test results for K-point grid in reciprocal space.

We performed convergence tests for the KPOINTS parameter. The test results are shown in Fig. S1. Specifically, the energy values of two different structures were calculated using different k-point meshes, and the energy difference between these structures was analyzed. Convergence was considered achieved when the relative error fell below 0.001 eV per atom. Ultimately, the k-point mesh was set to $3 \times 5 \times 5$.

Radial distribution function of single doped system

We calculated the radial distribution functions (RDFs) of C–C pairs for the B, O, and S mono-doped systems, respectively. Taking the carbon atoms within the first coordination shell of each dopant as centers, we statistically evaluated their average RDFs with all surrounding carbon atoms over a 1 ns period. For comparison, the corresponding results for pure diamond are also provided, as shown in Fig. S2. Due to the significant differences in atomic radii between O/S and C, doping with these elements induces notable lattice distortion, leading to a more pronounced leftward shift of the first peak position in the RDF compared to the B-doped system. Furthermore, the RDFs of the remaining coordination shells also show significant deviations from those of ideal diamond, primarily because O and S introduce

substantial local lattice distortions. In contrast, the atomic radius of B is similar to that of C, resulting in minimal lattice distortion upon doping; thus, the C–C RDF remains largely consistent with that of ideal diamond.

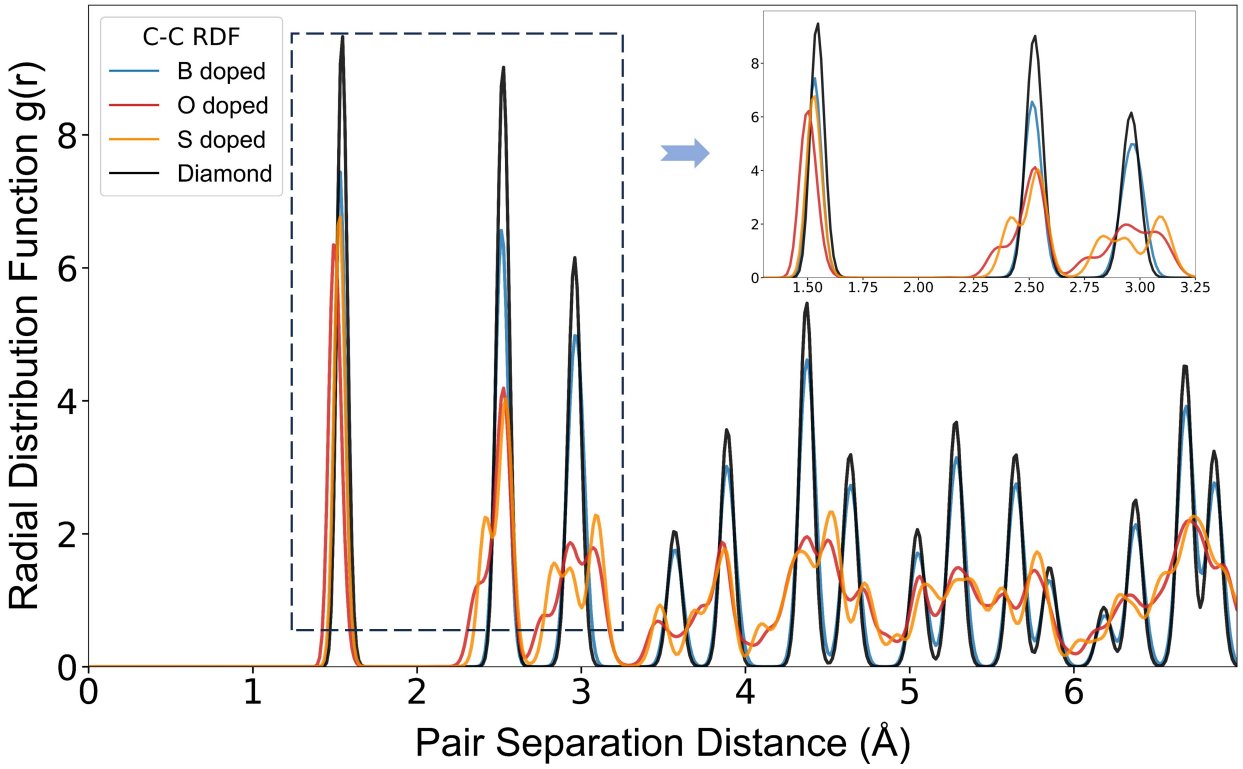

Figure S2: The average radial distribution functions (RDFs) of C–C pairs, centered on the carbon atoms within the first coordination shell of the B, O, or S dopant, calculated over a 1 ns timeframe. The RDF for perfect diamond is shown as a black line for comparison.

Radial distribution function of B-O co-doping

To further investigate the influence of B–O complex structures on the diamond lattice, we computed the C–C radial distribution functions (RDFs) in B–O co-doped systems with varying concentrations after hybrid MD/MC simulations. Following the same methodology, the carbon atoms within the first coordination shell of the dopants were taken as centers, and their average RDFs with all surrounding carbon atoms over a 1 ns period were statistically evaluated. As shown in Fig. S2, the C–C RDFs in these co-doped systems demonstrate closer agreement with the distribution profile of pristine diamond compared to those in B and O mono-doping structures. This result confirms that the complexes formed through hybrid MD/MC simulations effectively mitigate lattice distortion and enhance the structural integrity of diamond.

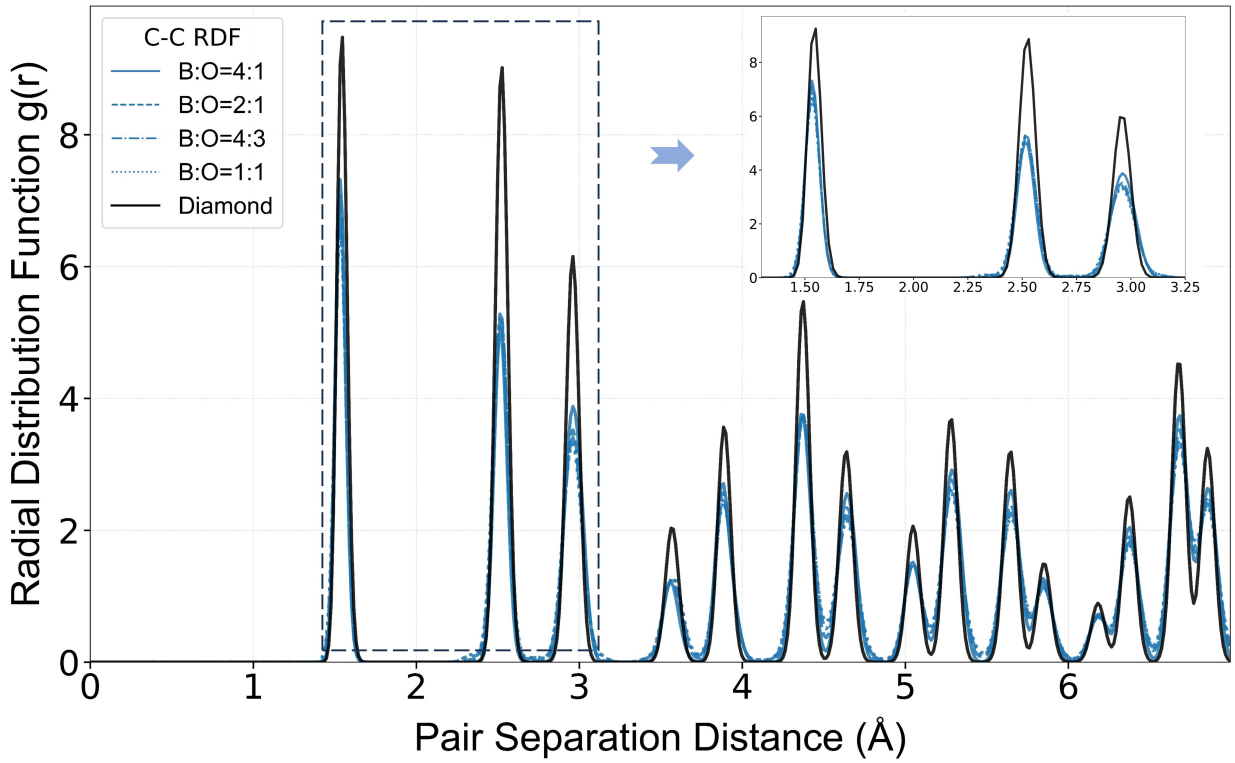

Figure S3: Radial distribution functions (RDFs) of C–C pairs centered on carbon atoms in the first coordination shell of B–O co-doped diamond.

Radial distribution function of B-S co-doping

We also calculated the radial distribution function (RDF) of the C-C pairs in the B-S co-doping system using the same procedure. As shown in Fig. S4, the RDF curve of this system is closer to that of ideal diamond compared to the case of S doping alone. This result indicates that the introduction of B atoms can effectively suppress the lattice distortion induced by S doping, thereby contributing to the restoration of the integrity of the diamond crystal structure.

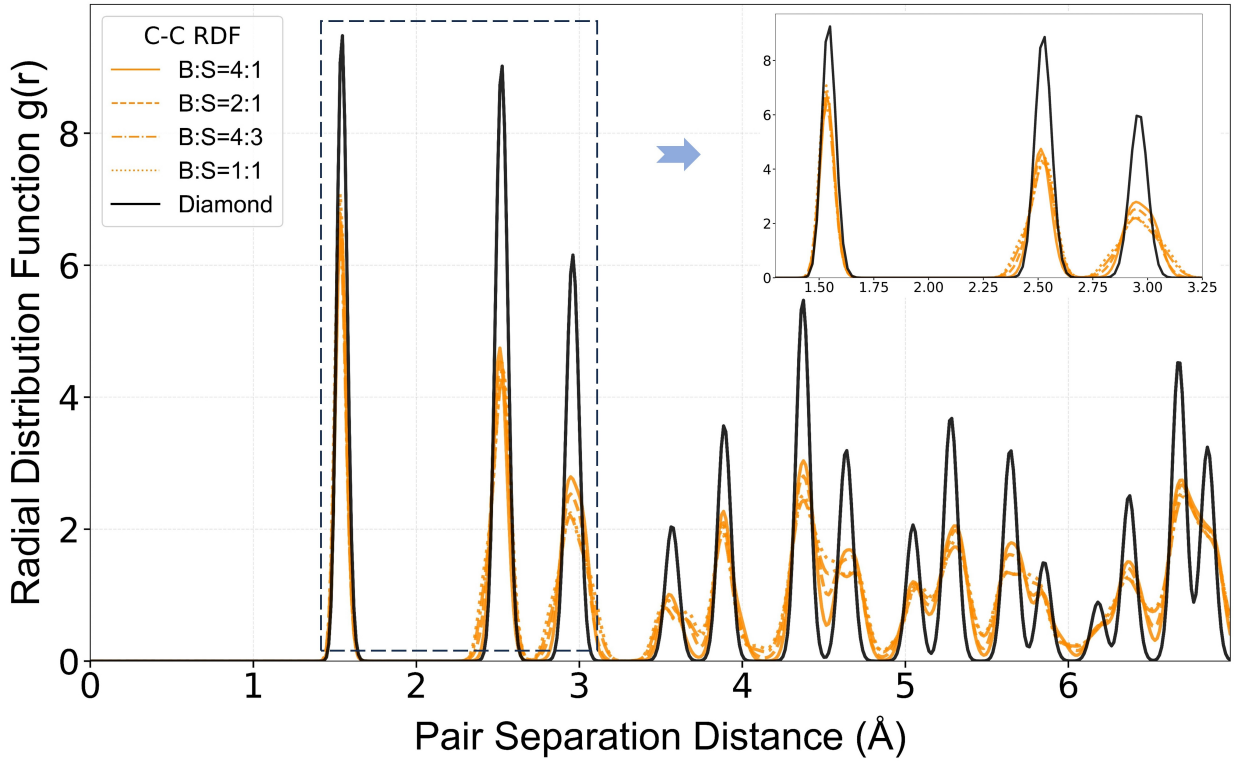

Figure S4: Radial distribution functions (RDFs) of C–C pairs centered on carbon atoms in the first coordination shell of B–S co-doped diamond.