Supporting Information for:


Mechanical properties of interfaces between Mg and SiC:

An *ab initio* study

In this supplementary material, we discuss the convergence tests made to determine the DFT parameters, using the CSi(111)Mg(0001) as an example.

### 1. Kinetic energy cutoff for wave functions

The parameter ecutwfc of Quantum ESPRESSO defines the kinetic energy cutoff for wave functions. As shown in the following Fig. S1, the total energy of the three different systems converges when the cutoff is set to over 40 Ry. Furthermore, the pseudopotential library also suggests a recommended ecutwfc value for each atom. The ecutwfc was set to 45 Ry after comprehensive consideration.
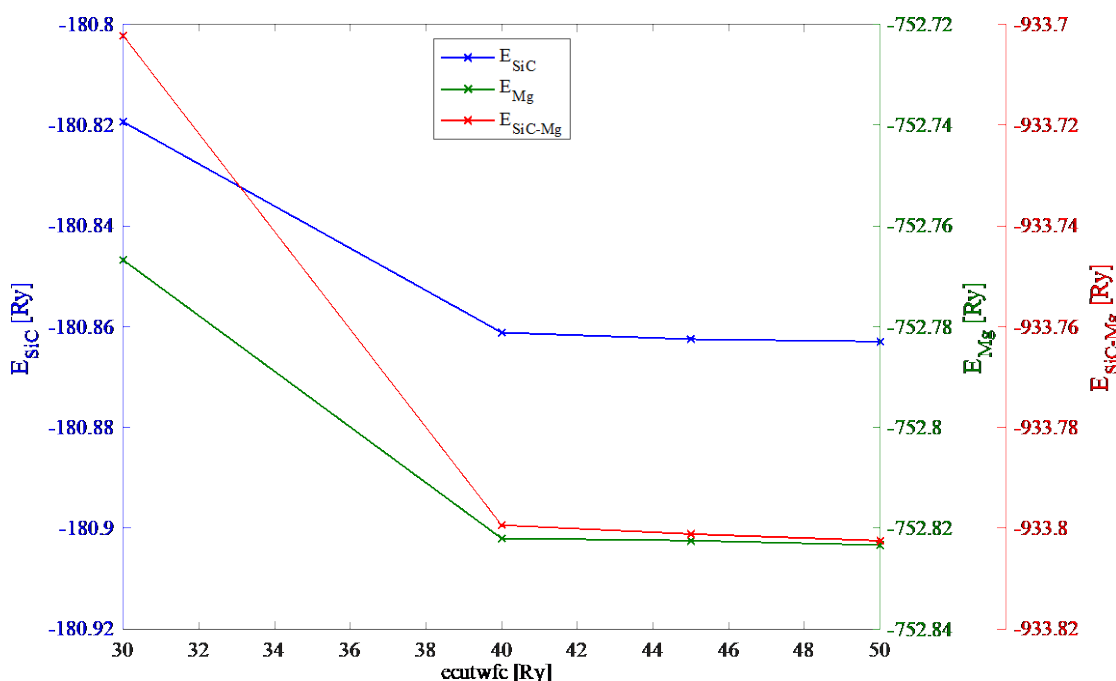
Figure S1. Convergence test of total energy, E, of SiC, Mg, and SiC-Mg with respect to kinetic energy cutoff for wave functions.

## 2. Kinetic energy cutoff for charge density and potential

The parameter ecutrho of Quantum ESPRESSO defines the kinetic energy cutoff for charge density and potential. As illustrated in Figure S2 below, the total energy of the three different systems converges when ecutrho is set to over 270 Ry. Furthermore, considering that ultrasoft pseudopotentials are used for Mg in our calculation, the value of ecutrho was set to 450 Ry, namely 10 times ecutwfc, to ensure stable calculations.
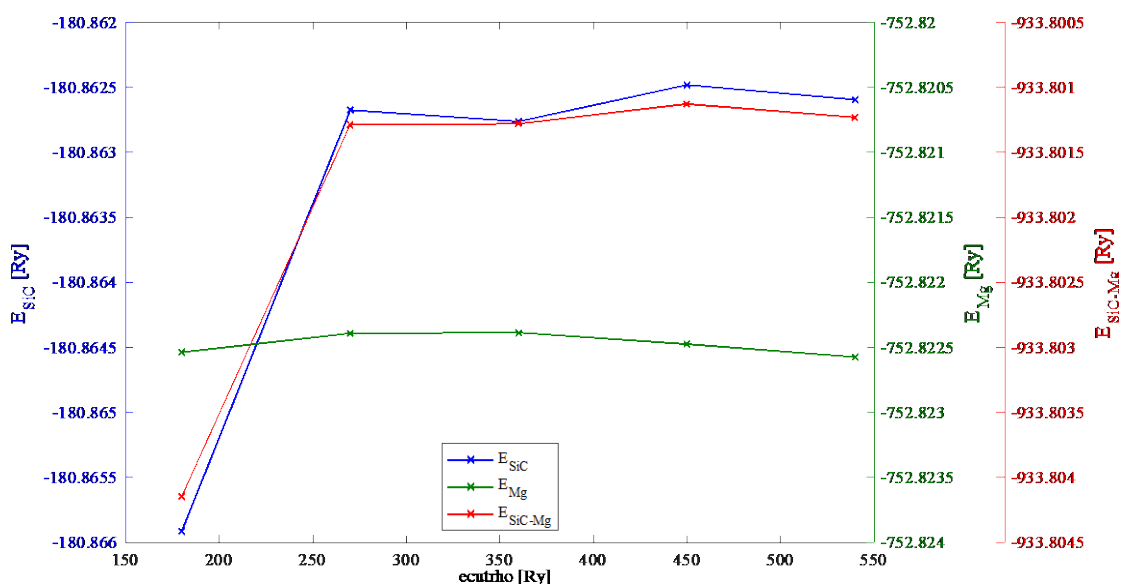
Figure S2. Convergence test of total energy, E, of SiC, Mg, and SiC-Mg with respect to different ecutrho value.

3. Number of k-points

Considering that the length of z-direction is much larger than the other two directions, the number of k-points in z-direction is fixed to 1. Fig. S3 illustrates that the total energy of the three respective systems converges when the k-points are set denser than 4×4×1. The convergence tests conducted for other structures also reach the same conclusion. A 6×6×1 k-point grid is used in the calculations for all configurations.
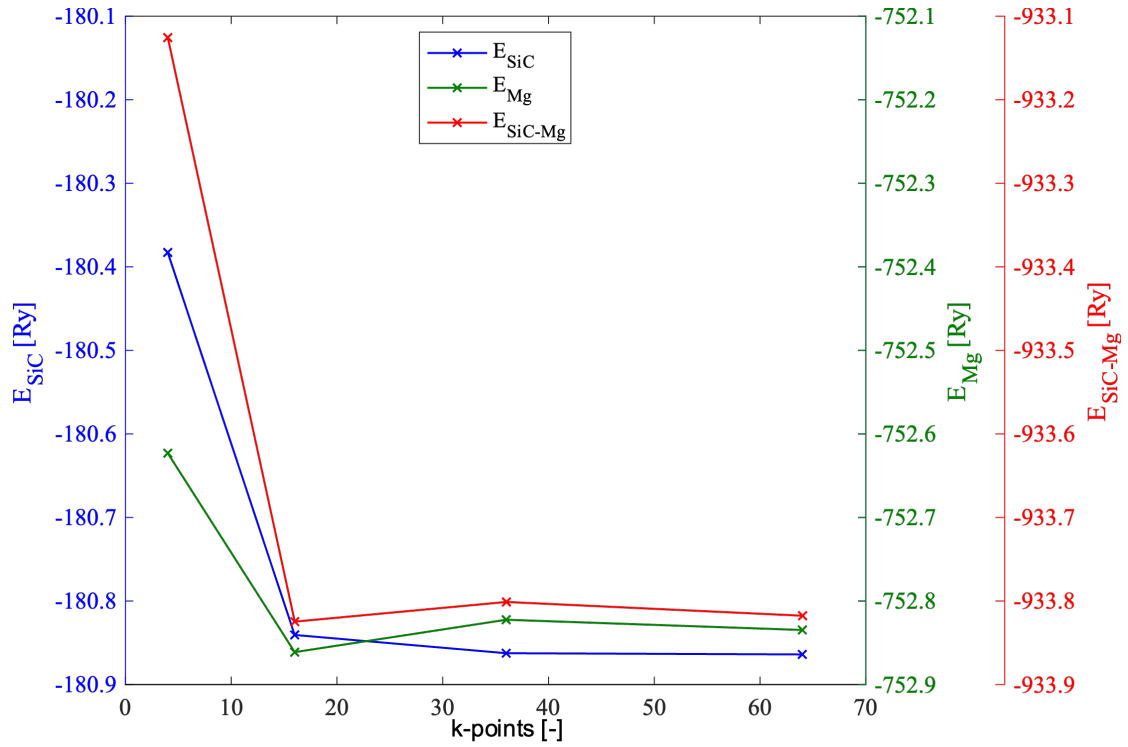
Figure S3. Convergence test of total energy, E, of SiC, Mg, and SiC-Mg with respect to varying k-point settings.