Supplementary material for the paper: "Diffraction of helium on MgO(100) surface calculated from first-principles"

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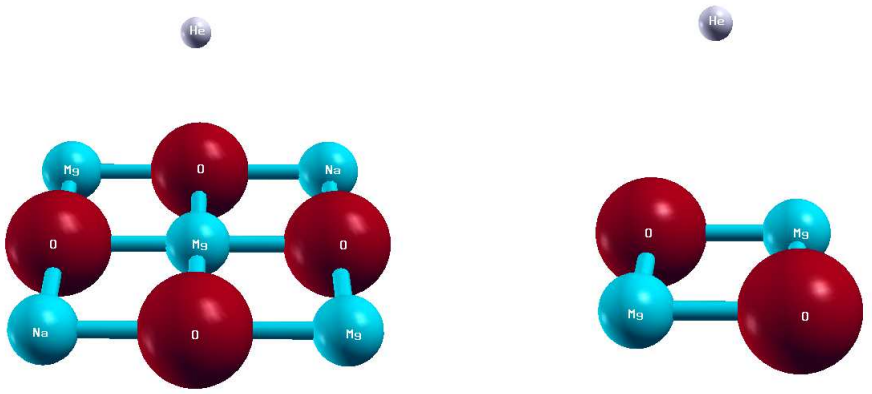
The clusters employed for evaluating the corrections are depicted in Fig. 1. The dimer He–$Na_2Mg_3O_4$ was used for the LMP2→CCSD(T) correction and the dimer He–Mg_2O_2 for the CCSDT(Q)-CCSD(T) energy difference correction. In both clusters the oxygen-metal distance was taken the same as in the MgO slab (2.105 Å).

In the local MP2 calculations on the He–$Na_2Mg_3O_4$ cluster, 8 ghost atoms were additionally added around the oxygen atoms, as is shown in Fig. 2. This allowed us to use similar LMP2 excitation domains as in the periodic LMP2 calculations. In the LMP2 calculations, the AOs of the Mg's AVTZ basis set (see Text for the specification) were used for the ghost atoms, as well for the sodium atoms.



(a) (b)

FIG. 1:
(a): He–$Na_2Mg_3O_4$ dimer used in the LMP2→CCSD(T) correction scheme;
(b): He–Mg_2O_2 dimer used for the CCSDT(Q)-CCSD(T) single point energy correction

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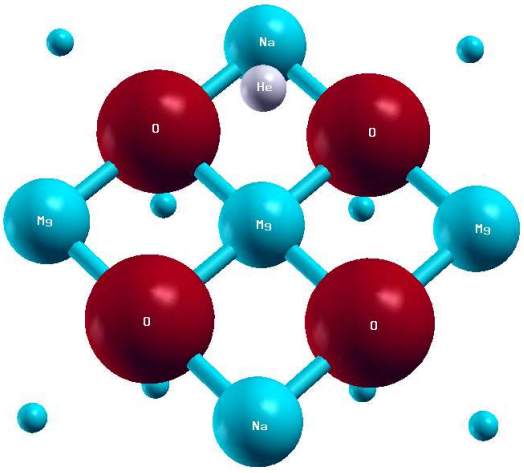

FIG. 2: The He–$Na_2Mg_3O_4$ dimer with the ghost atoms, holding the Mg's AVTZ basis functions, placed aside and below the oxygen atoms. The ghost atoms are given as small spheres. The positions of the ghost atoms correspond to the positions of the Mg atoms in the slab. In order to make the periodic and finite cluster LMP2 calculations compatible, in the latter the excitation domains for each localized orbital were chosen to include the ghost atoms closest to the oxygen, it was belonging to.