SUPPORTING INFORMATION

"Deprotonation and vacancies at $CH_3NH_3PbI_3$/ZnO and $CH_3NH_3PbI_3$/GaN, detected in the theoretical XANES"

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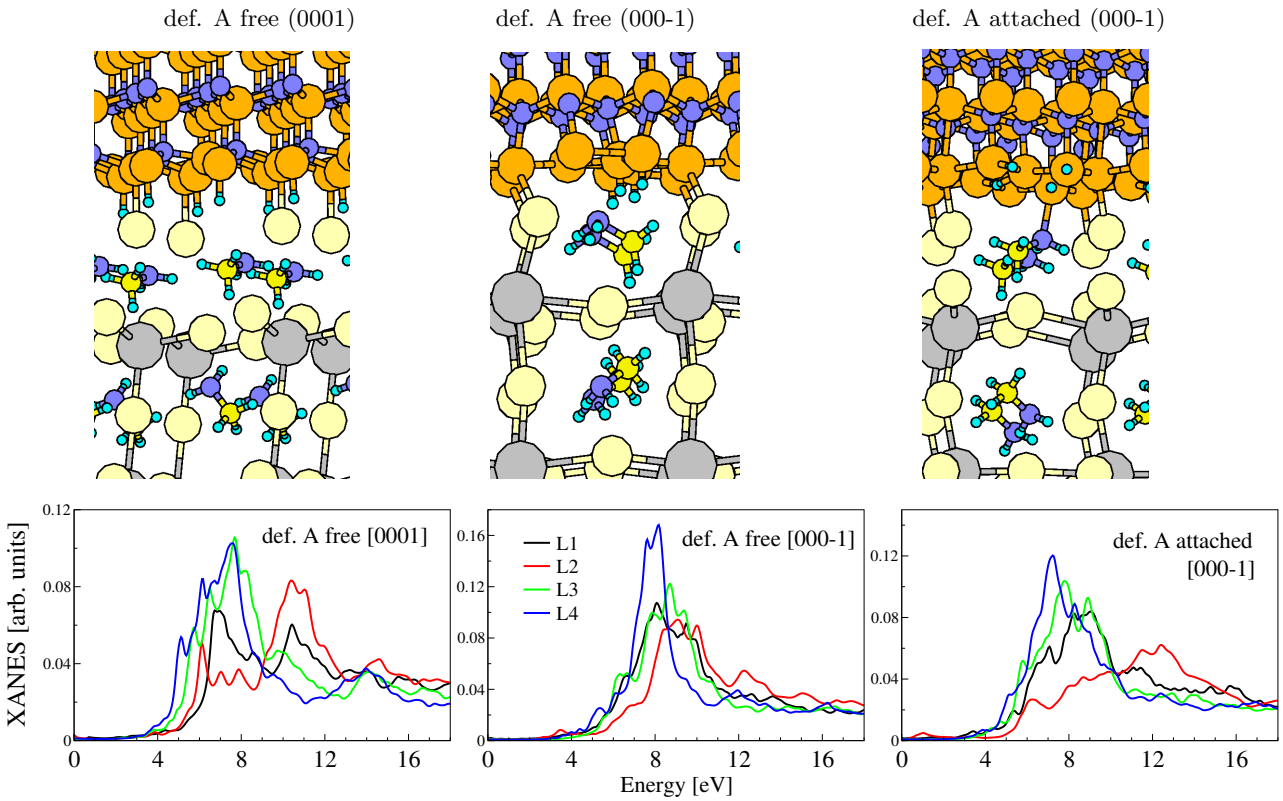

FIG. 1: The atomic structures and the XANES calculated for the A-type defected $CH_3NH_3PbI_3$ interfaced with GaN (0001) and (000-1). The CH_3NH_2 molecule in the first layer (L1) is either free or adsorbed at GaN.

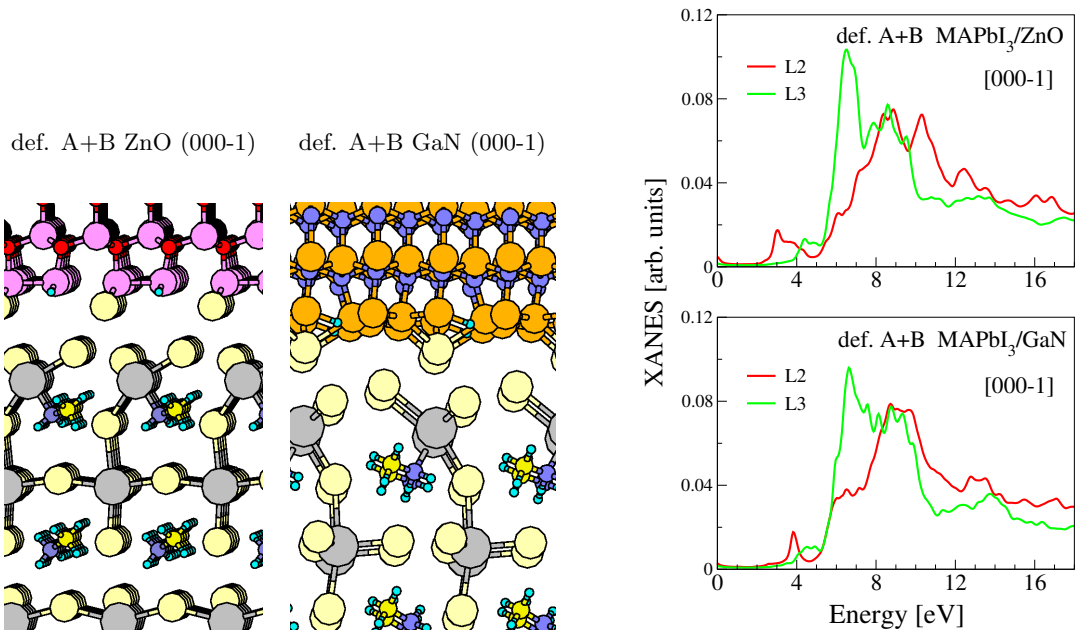

FIG. 2: Comparison of the atomic structures and the XANES for $CH_3NH_3PbI_3$ interfaced with ZnO and GaN (000-1) surface. The A-type defect in the second layer (L2) is combined with the B-type defect in the first and last layers (L1 and L4).

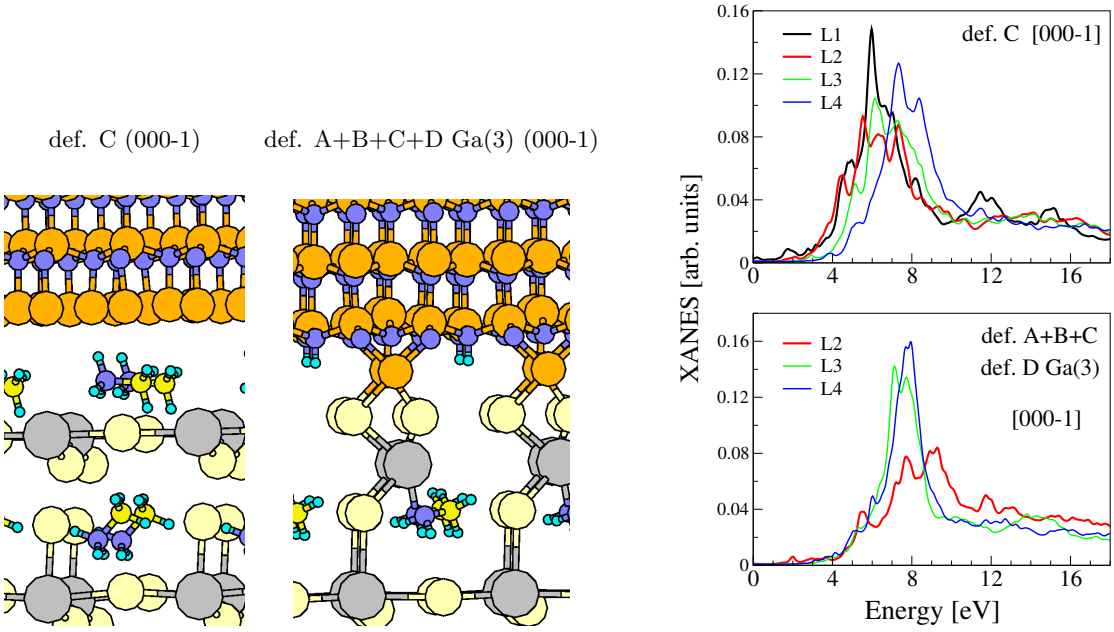

FIG. 3: The atomic structures and the XANES for the $CH_3NH_3PbI_3$/GaN (000-1) interface. The cases with the C-type defect and a combination of the defects A, B, C, and D (3-Ga vacancies).

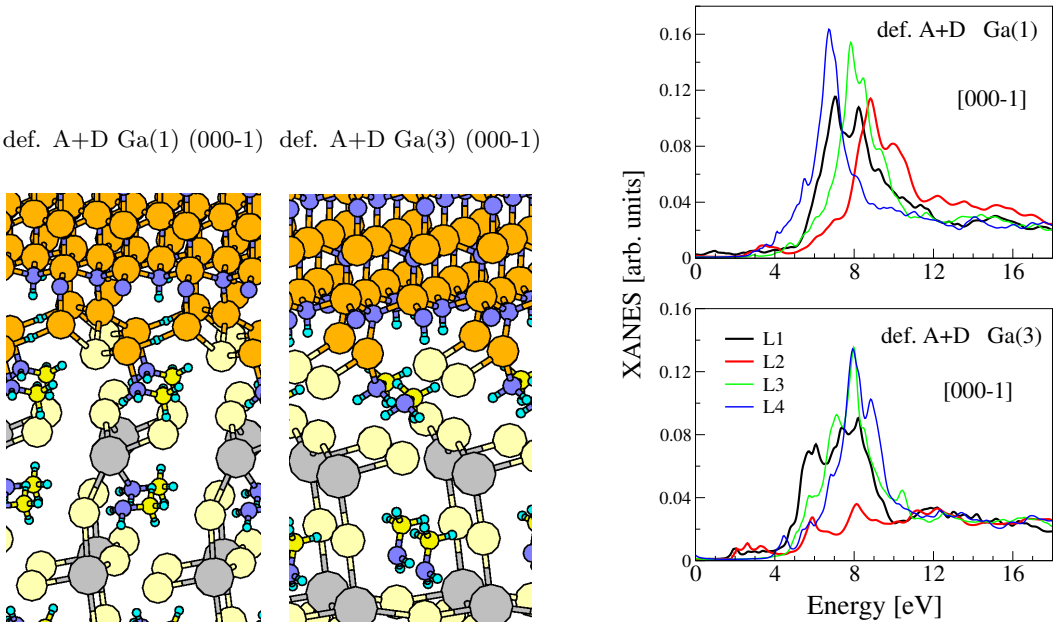

FIG. 4: The atomic structures and the XANES for the $CH_3NH_3PbI_3$/GaN (000-1) interface. The A-type defects in the first and second layers (L1 and L2) are combined with the D-type defect (either 1-Ga or 3-Ga vacancy).