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Band diagram of the $AlF_3/SiO_2/Si$ system

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The material system aluminum fluoride-silicon oxide-silicon ($AlF_3/SiO_2/Si$) can localize a high density of fixed negative charges in fluorine (F) vacancies within AlF_3, serving as a source for a strong drift field. This assignment is corroborated by a determination of the stoichiometry with Rutherford backscattering techniques and the transient response of the negatively charged defects with deep level transient spectroscopy. From the density-functional calculations of stoichiometric and understoichiometric AlF_3, we deduce a microscopic picture where the energetic eigenstates of the the singly and doubly occupied F vacancies surround the Fermi energy. The lineup of the band edges of the system $AlF_3/SiO_2/Si$ is determined by self-consistent electrostatic calculations including local charges, resulting in excellent agreement with the energetics deduced from the transient response of the charged defects.
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