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Dynamic dimer formation between superionic fluorines in CaF_2
MASASHI SAITO, TOMOFUMI TASAKA, KAZUO TSUMURAYA, Meiji University, Kanagawa, Japan — Recently we have elucidated the formation of the dynamic dimers in the conductor α-CuI through the analyses of the correlation peaks of the partial pair-distribution functions and the partial angle distribution functions with the first principles molecular dynamics (MD) method.(J. Phys. Soc. Jpn. 81,055603(2012).) The present study investigate the formation of the dynamic dimers and the migration paths of the dimers in the conductor CaF_2 with the MD method. The fluorines form the dynamic $32f$-$8c$ dimers with the coordinate (x,x,x) x=0.300. These incommensurate dimers allow to decrease the migration barriers of the fluorines.

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