Intrinsic self-diffusion of MgO by molecular dynamics simulation

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Intrinsic self-diffusion of MgO is simulated by molecular dynamics (MD) and self-diffusion coefficient under various temperature and pressure are expected. MD calculation is performed for MgO crystal with a pair of vacancy under the hypothesis that the pair vacancy migration mechanism dominates intrinsic self-diffusion of MgO. Calculated diffusion coefficient and its activation energy is homogeneous for experimental value of O above 2,000 K temperature when ordinary pressure.