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Ga Surface Diffusion on GaAs(001) β 2(2 $\times$ 4): An ab initio Local Superbasin Kinetic Monte Carlo Study[1] YANGZHENG LIN, KRISTEN FICHTHORN, Penn State University — We use first-principles density functional theory to characterize the diffusion of a Ga adatom on GaAs(01) β 2(2 $\times$ 4). Beginning with previously identified potential energy minima on this surface, we used the climbing-image nudged elastic band method to identify transition states and delineate diffusion pathways. These studies led to the discovery of eight new binding sites for Ga, which more than doubles the number that had been previously identified. The diffusion pathways for hopping between these minima involve energy barriers that vary significantly in magnitude, such that minima are spatially arranged in groups connected by low barriers and separated from each other by high barriers. Thus, the diffusion process is significantly more complex than was previously believed. To resolve the diffusion, we applied our recently developed local superbasin kinetic Monte Carlo method, which efficiently resolves the long-time dynamics of this complex process.

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