Surface reactions in the silicon PECVD process

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The Plasma enhanced chemical vapor deposition (PECVD) process is an important industrial process to produce solarcells and other semiconductor materials.
Understanding the growth process needs detailed understanding of the surface reactions. In the standard model of surface growth in the PECVD process the dominant precursor is the SiH_3 radical [1].
To get reaction rates for these reactions we calculated the minimum energy paths (MEP) of the elementary reactions of SiH_3 on the Si(111) surface with the nudged elastic band (NEB) method [2]. The saddle points were obtained by the DIMER method [3]. All calculations were done with DFT (GGA-PW91, PAW Pseudopotentials), plane wave basis sets and periodic boundary conditions [4].

References

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