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Explosive recombination-enhanced Re defect migration in MoS_2 WEIWEI SUN, Vanderbilt University, USA, SHIZE YANG, Oak Ridge National Laboratory, USA, YUYANG ZHANG, Vanderbilt University, USA, YONGJI GONG, PULICKEL M. AJAYAN, Rice University, USA, MATTHEW F. CHISHOLM, Oak Ridge National Laboratory, USA, WU ZHOU, University of Chinese Academy of Sciences, China, SOKRATES PANTELIDES, Vanderbilt University, USA — Via scanning transmission electron microscopy, substitutional Re impurities in MoS_2 are observed to undergo exchanges with neighboring Mo atoms on a time scale of several seconds. Density functional theory calculations of multiple possible diffusion pathways predict a large barrier that rules out thermal jumps and also rules out jumps induced by the electron beam because the energy transfer to Re is quite small. Microscopy further reveals that several S vacancies accompany Re atoms and that the initial and final configurations have different number and configurations of S vacancies. Density functional theory calculations find that the hydrogenic level of an isolated Re impurity becomes deep with small displacements of the Re atom and the S vacancies introduce additional deep levels so that the entire gap is filled with levels in constant motion. We propose that the observed jumps are the result of an "explosive" recombination-enhanced migration mechanism i.e., multiple electron-hole recombination events provide energy in multiples of the energy gap. The energy is transferred to local vibrations that ultimately cause the observed jumps.

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