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The interactions of bridging oxygen vacancies on the rutile (110) surface CRISTIAN CIOBANU, BRANDEN KAPPES, WILLIAM MADDOX, Colorado School of Mines, DANDA ACHARYA, PETER SUTTER, Brookhaven National Laboratory — Using density functional theory calculations at the level of Hubbard-corrected generalized gradient approximation (GGA+U), we calculate the formation and interaction energies of oxygen vacancies on the (110) surface of rutile for neutral and positively charged slabs for different values of the Hubbard parameter U. We find that the interaction of vacancies is elastically repulsive at long range, and that there is a short-range attraction between nearest neighbor vacancies (or oxygen vacancy pairs). With this physical description of the interactions, we derive a closed formula for the surface energy of reduced (110) rutile surface with two same-row vacancies within a given spatial periodicity along the bridge oxygen row, as well as a simple statistical mechanics description of the probability of finding two vacancies at a given distance d. The results of our theoretical model are consistent with our scanning tunneling microscopy determination of the distribution of intervacancy separations, and provide a framework for interpreting previous works in the literature.

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