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First-Principles Study of the Adsorption and Reaction of 2,3-Butanediol on Si(001)

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The adsorption and reaction of 2,3-butanediol on the Si(001) surface are investigated by first-principles density-functional calculations within the generalized gradient approximation. We consider the two different reaction pathways forming adsorption on top of a single dimer (termed the "on-top" structure) and across the ends of two adjacent dimers in the same dimer row (termed the "end-bridge" structure). For both reaction pathways, the O atom of the hydroxyl group initially bonds to the down Si atom of the buckled dimer and subsequently O-H dissociation takes place. However, the reaction of another hydroxyl group shows a drastic difference between the two reaction pathways. Along the former reaction pathway it is difficult to form the second Si-O bond because of a repulsive interaction between an O lone pair and a single Si dangling bond, thereby prohibiting formation of the on-top structure. On the other hand, along the latter reaction pathway an O lone pair of the hydroxyl group is attracted to the down Si atom of neighboring dimer, proceeding to formation of the end-bridge structure. These results provide an explanation for a recent scanning tunneling microscope observation that 2,3-butanediol occupies predominantly the end-bridge structure.