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Reply to Harold H. Kung

In the previous letter (*1*), Kung has raised questions concerning symmetry restrictions on surface reactions which are not properly treated within the framework of the crystal-field surface orbital–bond energy bond order model (*2*). The latter is an empirical model and, consequently, open to numerous theoretical criticisms (*3*). However, we do not feel that orbital symmetry is a serious restriction. It is well known that substrate band mixing occurs to a *very* considerable extent, even in the case of nonbonding molecular orbitals or admolecules, with energy levels which fall within the substrate valence band (*4–6*). Consequently, the conclusion of Kung that "Most molecular orbitals are largely preserved" is incorrect, as are his arguments concerning the generality of preserving orbital symmetry in *surface* reactions. It is recognized that orbital symmetry could be important in certain surface reactions, but, once symmetry-allowed pathways are identified, then the BEBO methods could presumably be applied to them as well. Unfortunately, it is not yet obvious how to identify when the orbital symmetry conditions should be invoked for surface reactions.

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