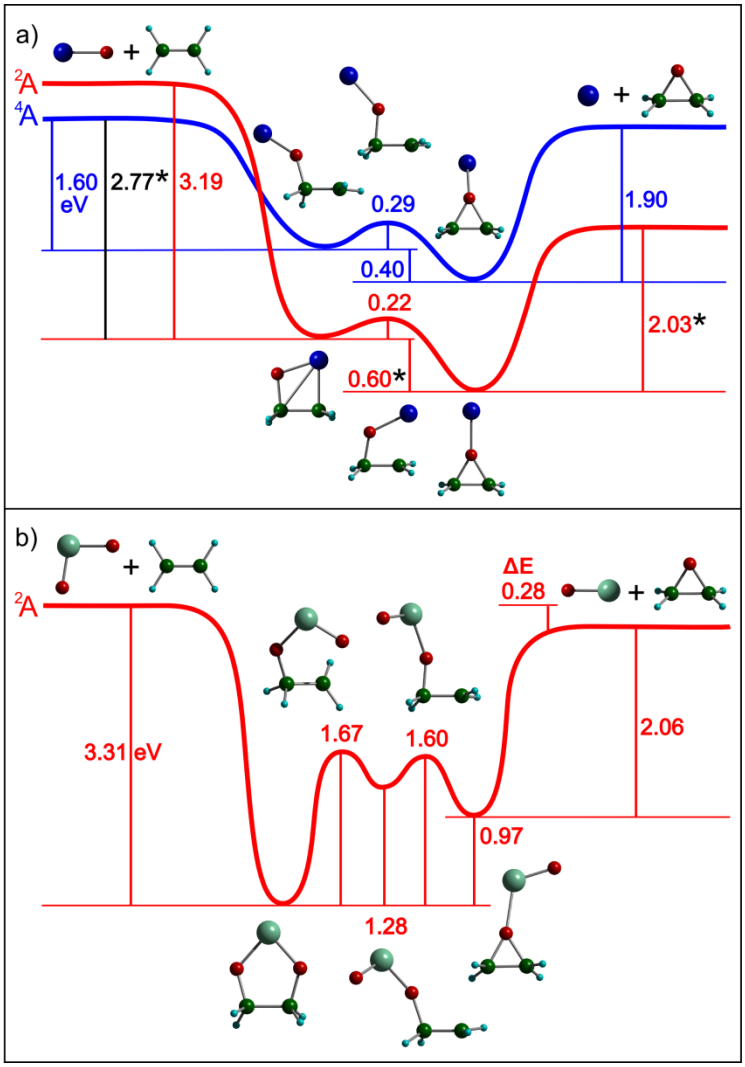
Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Exploring Similarities in Reactivity of Superatom Species: A Combined Theoretical and Experimental Investigation

Eric C. Tyo, Melanie Nößler, Sabine Rabe, Christopher L. Harmon, Roland Mitrić, Vlasta Bonačić -Koutecký*, and A. Welford Castleman, Jr.*



Supporting Information Figure S1. Calculated reaction profiles for oxidation of C_2H_4 to ethylene oxide by a) NiO^+ and b) TiO_2^+. The doublet and quartet state profiles are presented for interaction of NiO^+ with C_2H_4. Reaction in both states is exothermic by 1.76 eV and 0.10 eV, respectively. The energy differences labelled by * allow for the determination of the most favourable reaction energy by undergoing a spin-crossover which is exothermic by 1.34 eV. The exothermic energy difference ΔE for TiO_2^+ is shown in b).

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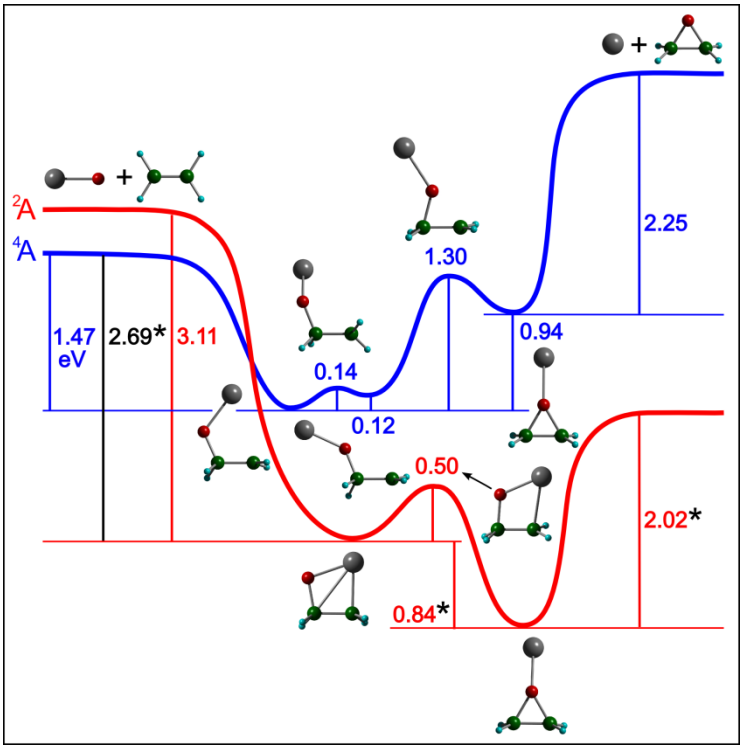

Supporting Information Figure S2. Calculated reaction profile for oxidation of C_2H_4 to ethylene oxide by PdO^+. Profiles for doublet and quartet states are shown. The reaction is exothermic by 1.93 eV in the doublet state and endothermic by 1.72 eV in the quartet state. The energy differences labelled by * allows for the determination of the most favourable reaction energy by undergoing a spin-crossover which is exothermic by 1.51 eV. (Creation of ethylene oxide through interaction of ethene and ZrO_2^+ is an endothermic process and as such the reaction profile has not been included.)