

Achieving tunable chemical reactivity through photo initiation of energetic materials at metal oxide surfaces

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Supplementary Information

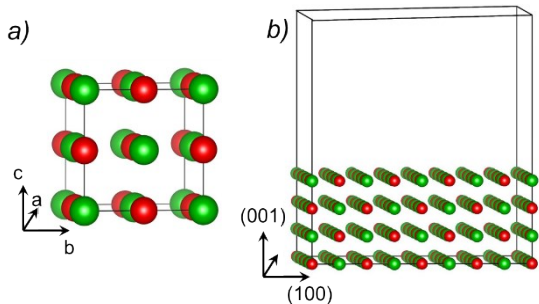


Figure S1. The Structures of MgO a) cubic crystalline lattice and b) periodic supercell slab model of the (001) surface. Mg atoms are shown in green, O atoms are in red.

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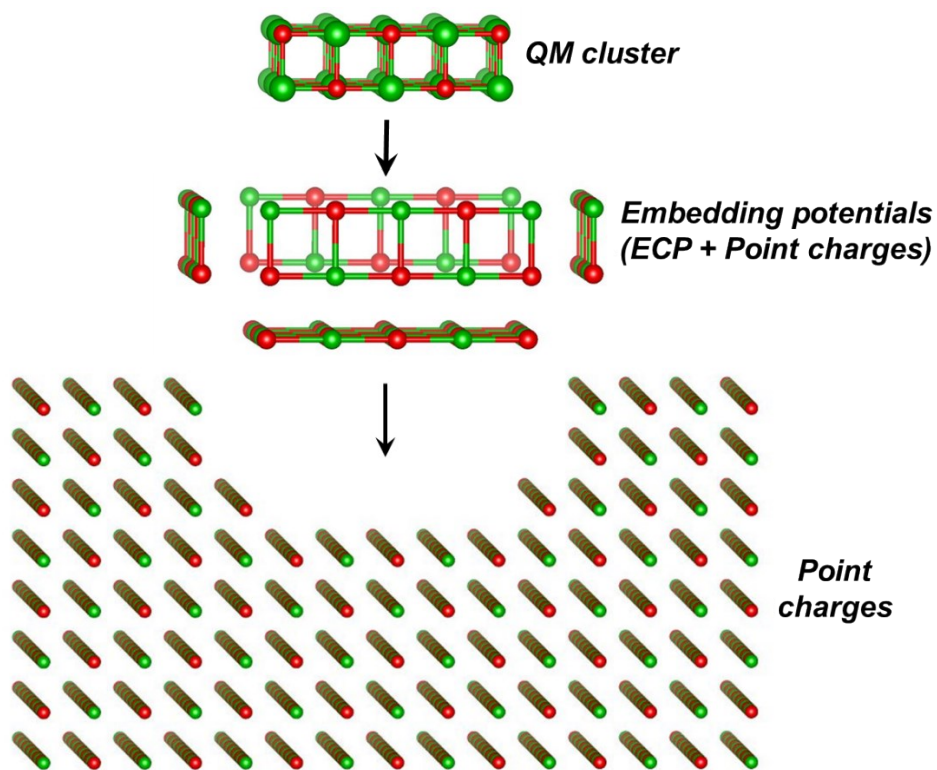


Figure S2. Schematic representation of the embedded cluster model, showing the quantum mechanical cluster, quantum cluster boundary, and the field of point charges that represent a MgO crystal. Mg atoms are shown in green, O atoms are in red.

Table S1. The calculated energies of the vertical ionization potential (IP), first singlet-singlet transition (S_0 - S_1), and HOMO-LUMO gap of MgO compared with previous experiments and theory.

MgO	This study	Reference	
		DFT	Exp. ^c
IP, eV (B3LYP)	6.46	6.7 ^a	6.2
S_0 - S_1 , eV (TD B3LYP)	5.00	5.3 ^b	5.5
HOMO-LUMO, eV (B3LYP)	5.65	-	5.5

^a from ref. ¹; ^b from ref.²; ^c from ref.³

Handling high explosive materials

Warning! PETN and TNT belong to a class of hazardous high explosive materials and can cause an explosion if exposed to heat or pressure. Hence, the materials have to be handled with caution.

Despite very small amounts of the EM in the actual experimental samples, it is necessary to carry out all the experimental manipulations with great care according to safety recommendations^{4,5,6,7} and using means of protection. Sonication and pressing of the samples were performed under the protective shield. The pressing matrix must be able to withstand an accidental explosion of the pressing sample without destruction. The Q-switched laser must be used according to safety regulations and recommendations for 4 class lasers. After a successful sample initiation, there are shards and crumbs of the glass cover in the explosion chamber. It can cause injury. The chamber has been cleaned after each test with a vacuum cleaner.

References

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- ¹ P. V. Sushko, A. L. Shluger, C. Richard, A. Catlow, *Surf. Sci.*, 2000, **450**, 153-170.
 - ² P. V. Sushko, J. L. Gavartin, A. L. Shluger, *J. Phys. Chem. B*, 2002, **106**, 2269-2276.
 - ³ P. A. Cox, A. A. Williams, *Surf. Sci. Lett.*, 1986, **175**, L782-L786.
 - ⁴ https://www.ilo.org/dyn/icsc/showcard.display?p_lang=en&p_card_id=0967&p_version=2
 - ⁵ https://www.ilo.org/dyn/icsc/showcard.display?p_lang=en&p_card_id=1576&p_version=2
 - ⁶ <https://pubchem.ncbi.nlm.nih.gov/compound/Pentaerythritol-tetranitrate>
 - ⁷ <https://pubchem.ncbi.nlm.nih.gov/compound/8376>