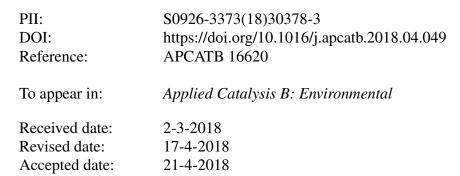
#### Accepted Manuscript

Title: The role of iron-oxide aerosols and sunlight in the atmospheric reduction of Hg(II) species: A DFT+U study

Authors: Sean A. Tacey, Tibor Szilvási, Lang Xu, James J. Schauer, Manos Mavrikakis



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### ACCEPTED MANUSCRIPT

# The role of iron-oxide aerosols and sunlight in the atmospheric reduction of Hg(II) species: A DFT+U study

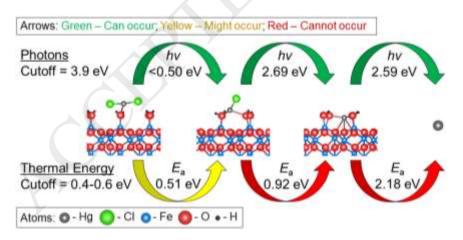
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#### **Graphical Abstract**



Highlights

- Gas-phase photochemical reduction of HgCl<sub>2</sub> and HgBr<sub>2</sub> is not possible in troposphere
- Phase diagrams determine stable iron-oxide surfaces under tropospheric conditions
- Thermal effects alone cannot promote mercury reduction on iron-oxide aerosols

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