Research Experiences for Teachers

# A computational analysis of the energy requirements for the reduction and re-emission of mercury chloride in the arctic


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## Phenomenon

- Bioaccumulated levels of various mercury species occur at a higher incidence in arctic animal and human populations compared to other large scale geographic regions on Earth.

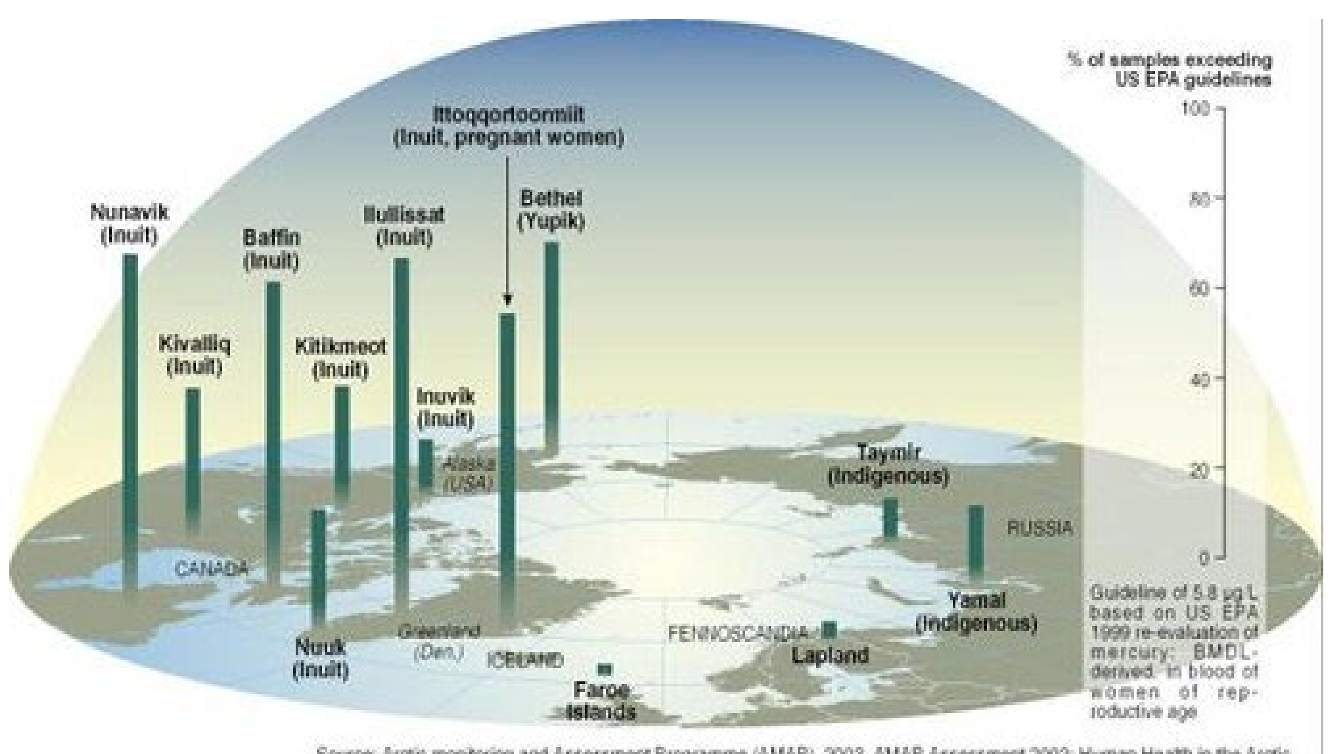


Figure 1: relative mercury levels in indigenous women of the arctic

- The sources, oxidation, and deposition of elemental mercury species and compounds has been widely studied.

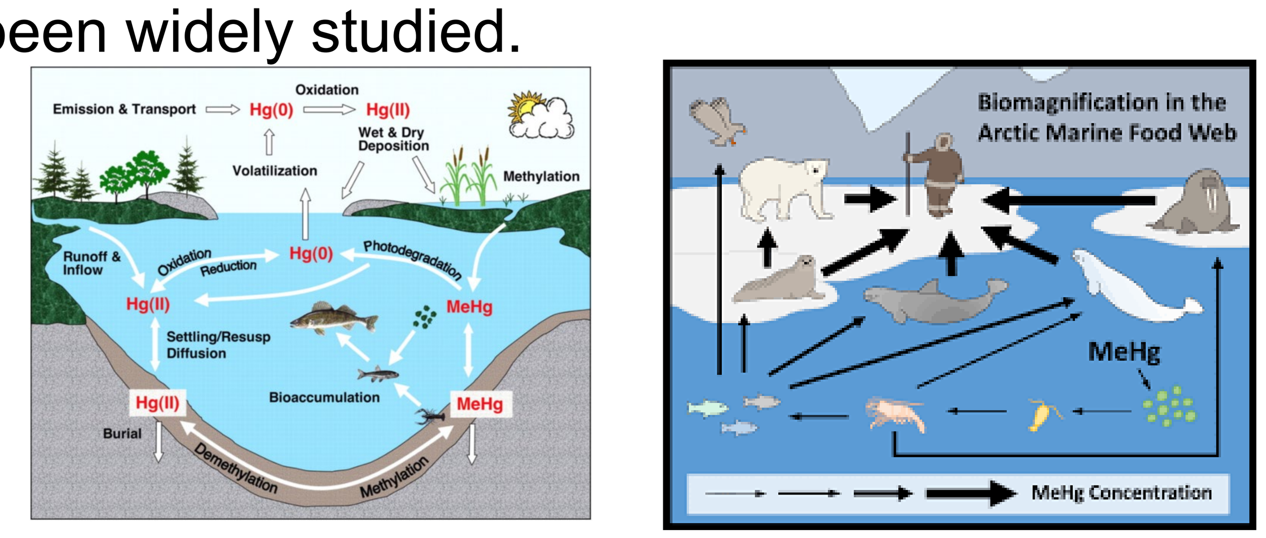


Figure 2: (A,Left) flow chart of mercury speciation in an aquatic environment (B, Right) flow chart of bioaccumulation of mercury in the arctic environment (source enviro wiki)

- The exact nature of the circulation of this deposited mercury is unknown and is the subject of our study.

## Research Question

What is the required energy to chemically reduce, and dissociate mercury chloride from an ice lake surface environment, as distance increases from the ice surface?

## Relevance

- Elemental mercury and its various forms are bioaccumulated and biomagnified in the arctic.
- Predator species in the arctic have high levels of mercury toxicity.
- Indigenous populations that rely on sustenance hunting of these species are at risk of the health impacts of this mercury, which is a neurotoxin.

## Research Methods

- Beginning with a model of the crystal lattice of an ice lake surface, we build in the deposited mercury chloride molecule, bonded to the ice surface.

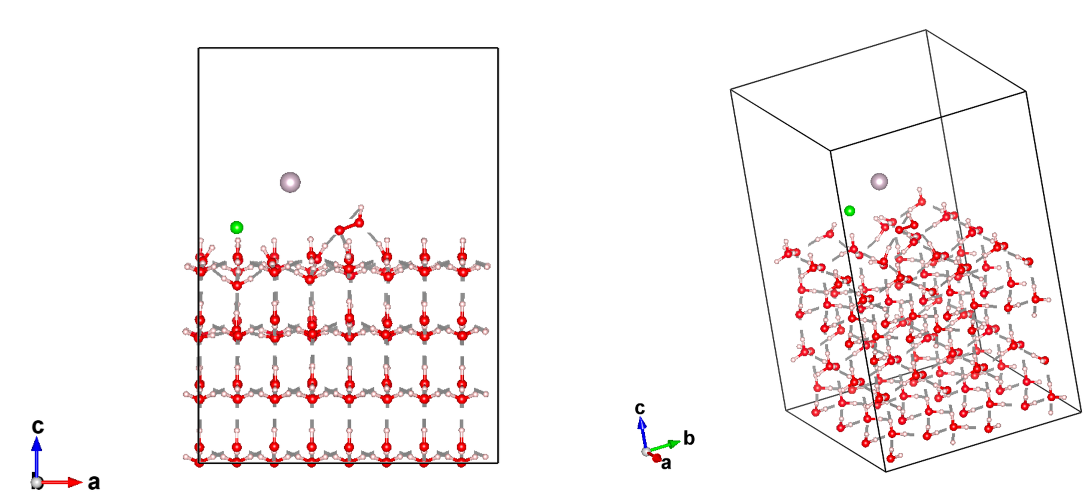

Figure 3: two perspective views of the ice crystal lattice with the mercury atom (white) and the chlorine atom (green).

- From the model data such as position, electron/charge density, and bonding types are exported out.

| | | | | | |
|---|---|---|---|---|---|
| 0.8778783783783766 | 0.9817870655452978 | 0.0268834281072330 | F | F | F |
| 0.5330176265483997 | 0.5265517354532346 | 0.6201498293352803 | T | T | T |
| 0.2920531316475575 | 0.5199080968991319 | 0.8361907540064379 | T | T | F |
| 0.1419520013366540 | 0.4483352024085340 | 0.6374774907836271 | T | T | T |

Figure 4: Three-dimensional position data from 4 atoms including the mercury and chlorine atoms.

- Utilizing VASP code, and access to the Penn State ROAR Collaborative super-computer complex we compute the energies required to pull the molecule away from the crystal lattice, working against the electrostatic forces of the molecular bond.
- Using UNIX commands, the position variables were altered, and the computations were sent to the ROAR Collaborative to be completed

## Data

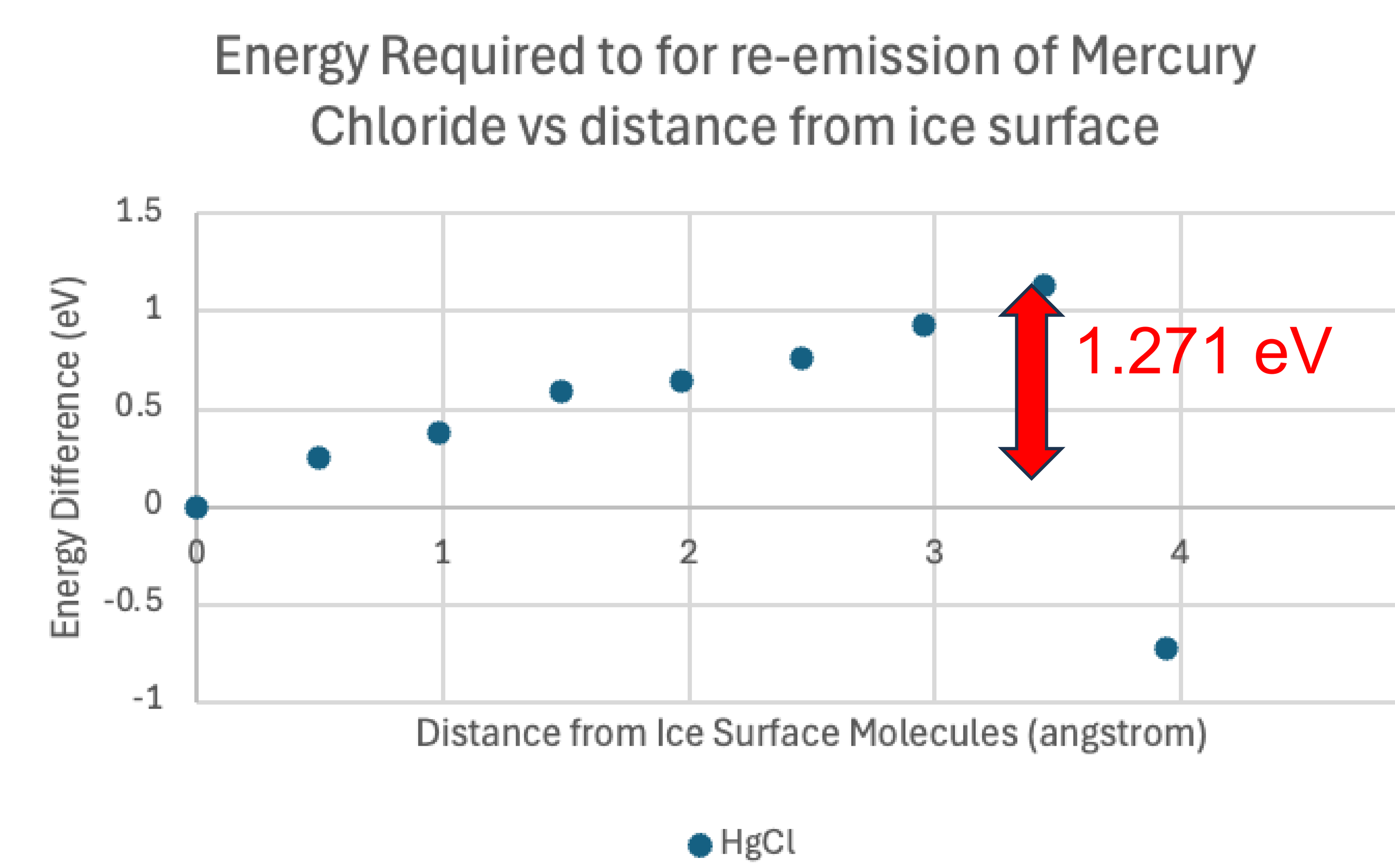


Figure 5:Scatter plot of Energy differences vs distance as HgCl molecule is pulled from ice surface.

## Analysis

- The energy required to remove the HgCl molecule was computed to be approximately 1.13 eV.
- Solar photon energy ranges from approximately 1.6-13 eV.
- HgCl requires an energy lower than available solar energy for reduction and re-emission.
- HgCl where present may easily contribute to the re-circulation of mercury in the arctic.

## Bibliography


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2. Vogelsong, L., Fuentes, J. D., & Asaduzzaman, A. (2023). Deposition and Reduction of Oxidized Mercury on the Ice Surface: QuantumChemical Study and Implication of Mercury Activities in the Arctic. Journal of Physical Chemistry C, 127(5), 2657- 2665. https://doi.org/10.1021/acs.jpcc.2c07879



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