

A computational analysis of the energy requirements for the reduction and re-emission of mercury from ClHgO_2H in the arctic.

Joel May¹, Abu Asaduzzaman²

¹North Tonawanda High School, North Tonawanda NY, ²Penn State Harrisburg School of Science, Engineering and Technology

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.

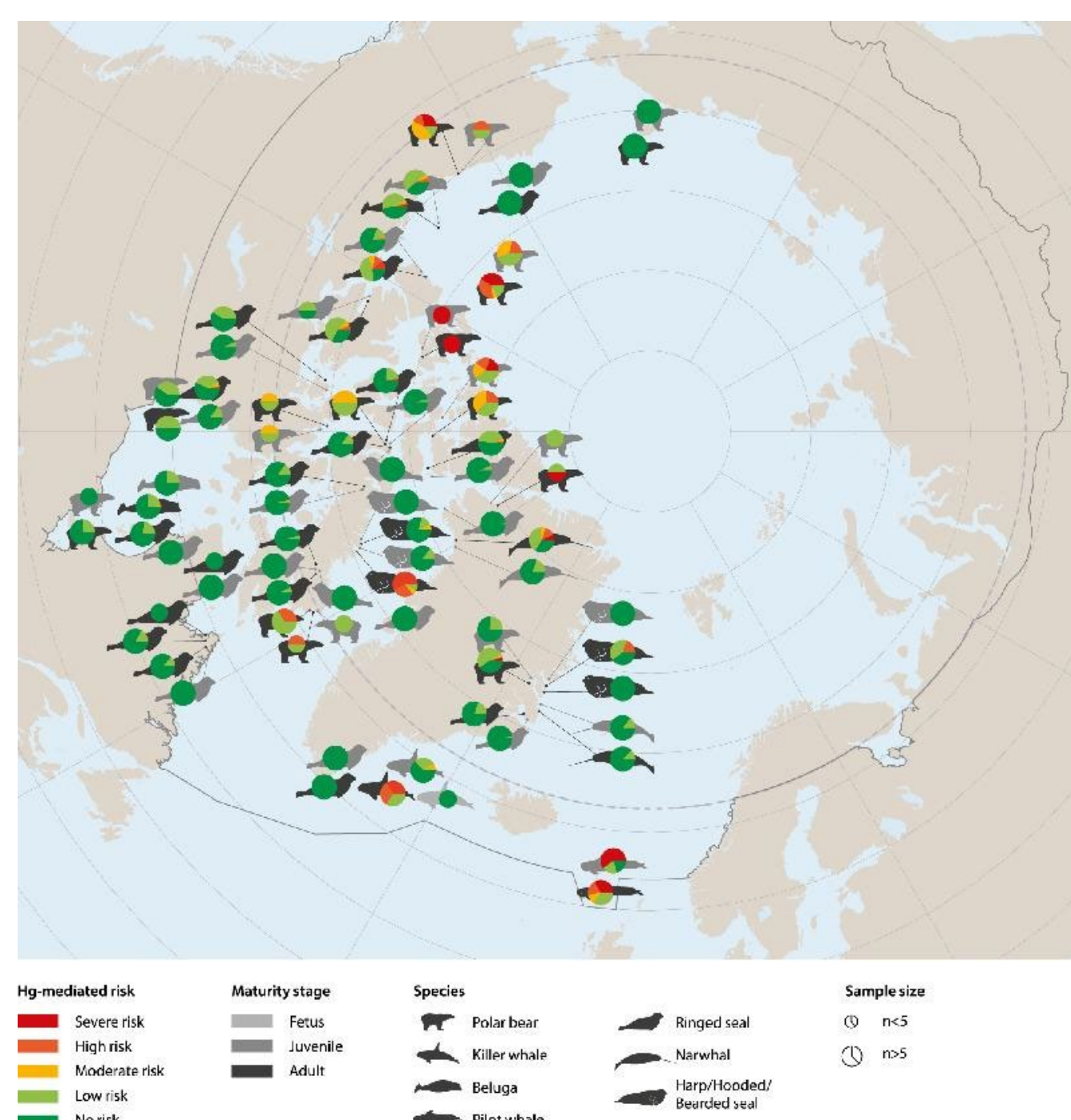


Figure 1: Relative Mercury Risk in Arctic Marine Mammals (source AMAP)

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

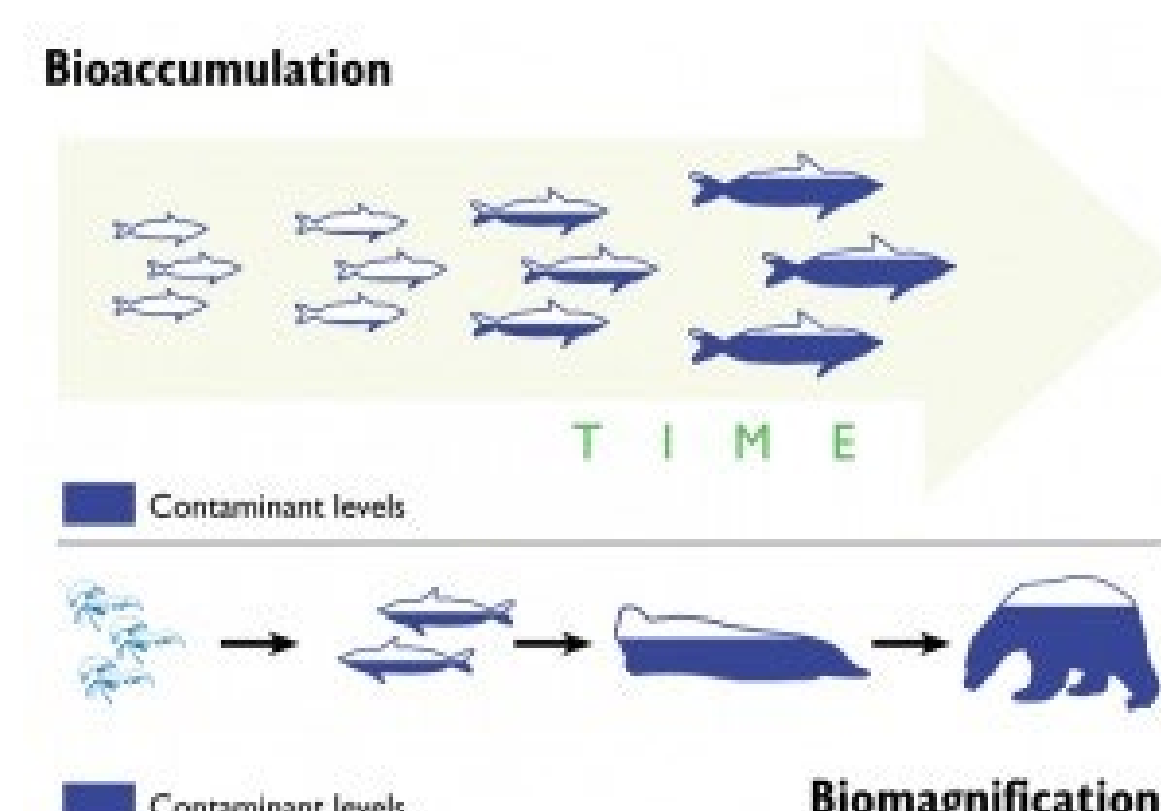


Figure 2: representation of bioaccumulation and biomagnification of mercury (source MIT)

- 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 from the ClHgO_2H molecule 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 built in the deposited ClHgO_2H molecule, bonded to the ice surface.

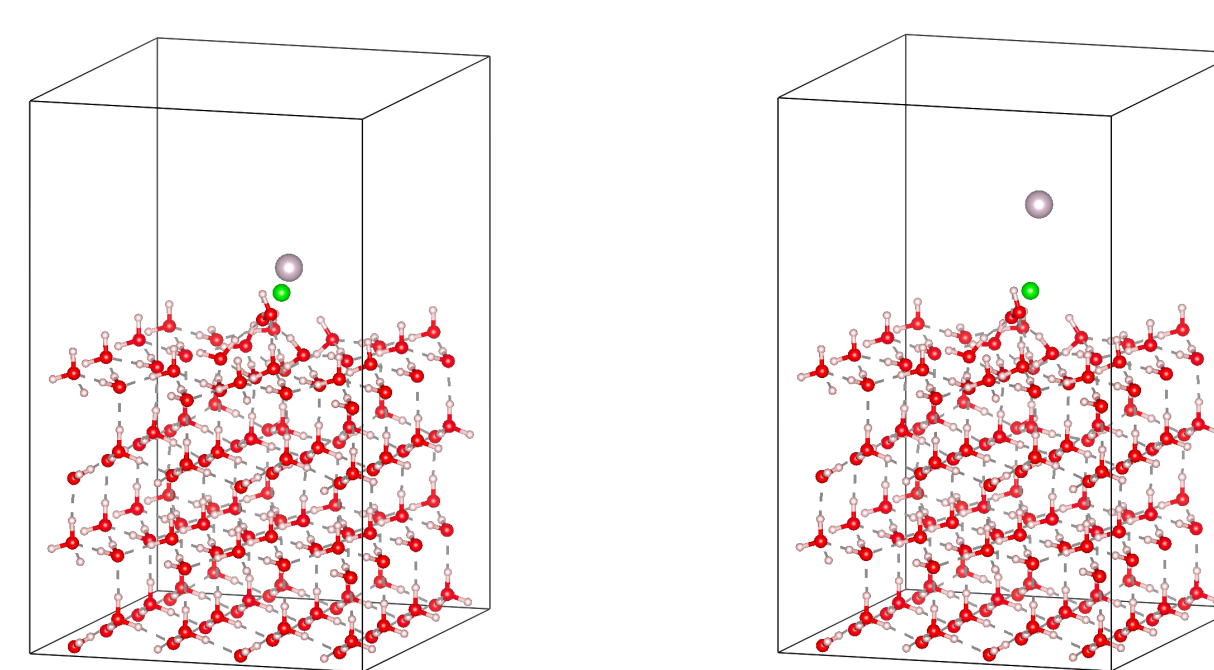


Figure 3: two perspective views of the ice crystal lattice with the mercury atom (white) and the chlorine atom (green) and the O₂H member (2 red and white)

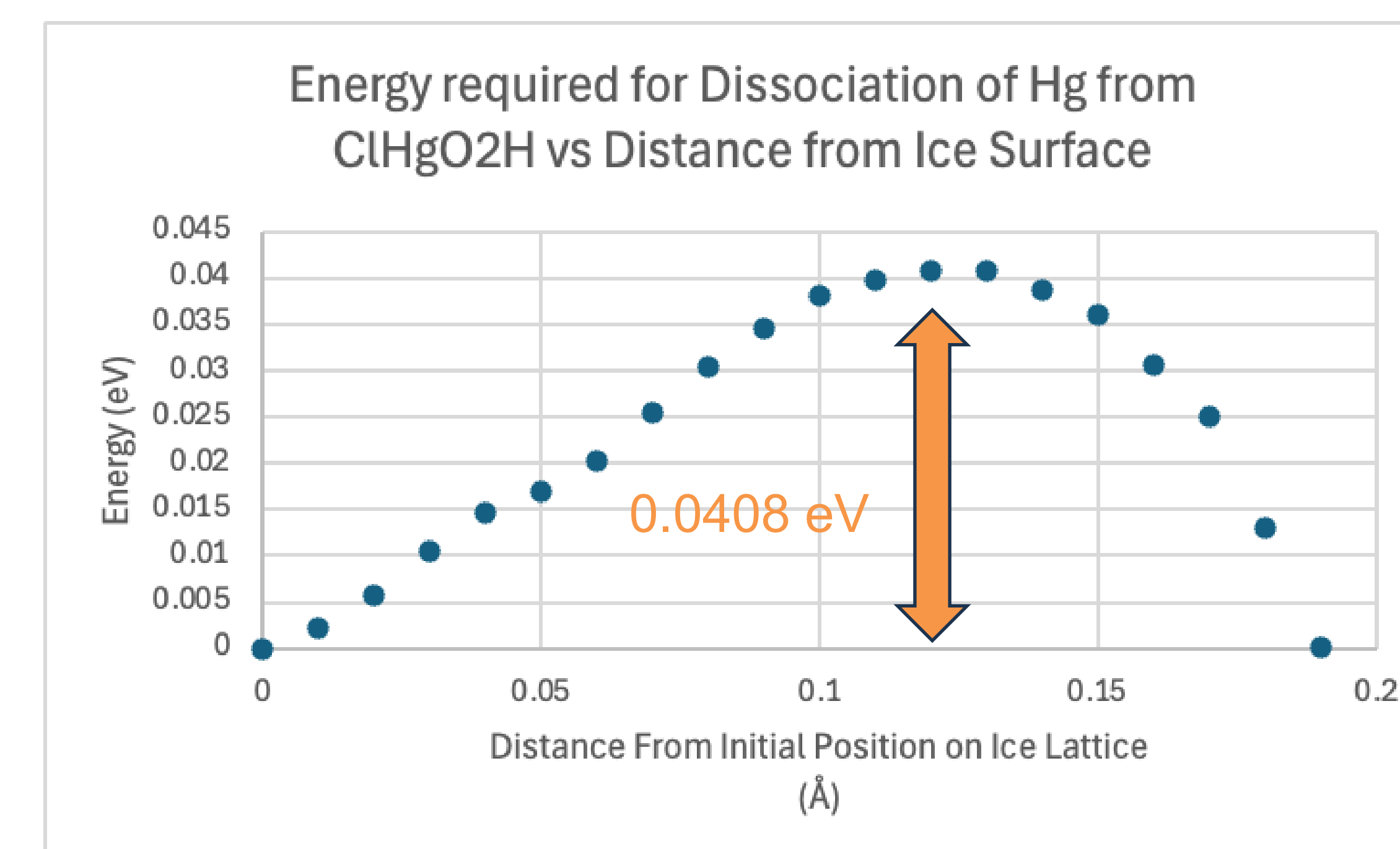
- From the model, data such as position, electron/charge density, and bonding types are exported out.

| | | | | | |
|--------------------|--------------------|--------------------|---|---|---|
| 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 the Penn State ROAR Collaborative supercomputer 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



Analysis

- The maximum energy required to remove mercury from ClHgO_2H is 0.0408 eV.
- Solar photon energies range from ~ 0.35 -5 eV and therefore contain enough energy to transfer to the mercury atom to remove it from the ClHgO_2H molecule in a collision.
- ClHgO_2H can readily contribute to the re-emission of elemental mercury into the atmosphere and can lead to recirculation in the arctic environment.
- Mitigation of the sources and processes that lead to the emission of ClHgO_2H should be considered to avoid a persistent source of mercury pollution.

Bibliography

- Amin, S., Asif, T., Khan, M., Usinowicz, E., Mitra, D., & Asaduzzaman, A. (2021). Structural, energetic and vibrational properties of oxidized mercury in the gas and aqueous phases. *Computational and Theoretical Chemistry*, 1198, 113186.