On the Trapping of Bjerrum Defects in Ice I_h: The Case of the Molecular Vacancy

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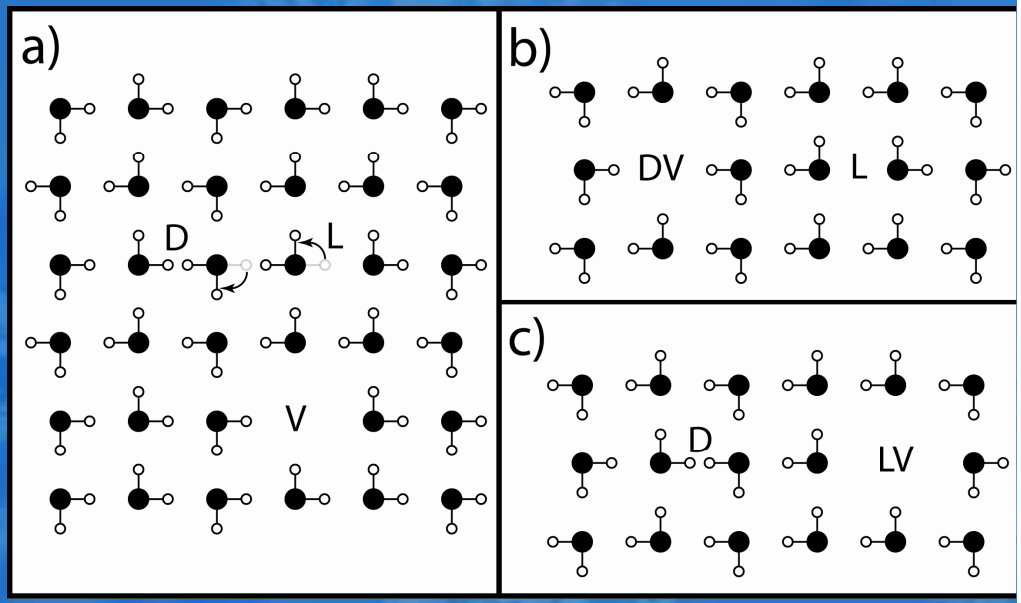
Motivation:

- Bjerrum defects play central role in electrical properties of Ice.
- Two species of Bjerrum Defects: D and L.
- Experimental evidence indicates that only L defects are mobile. Why?
- D defects trapped at other defects? : Molecular vacancy (Petrenko & Whitworth, "Ice Physics", OUP 1999).



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Objectives/Methodology:

- Compute intrinsic D-defect migration barriers.
- Study D/L+Vacancy complexes.
- DFT (VASP code). 96-molecule supercell. Nudged-elastic band (NEB) method. Different replicas of defects.

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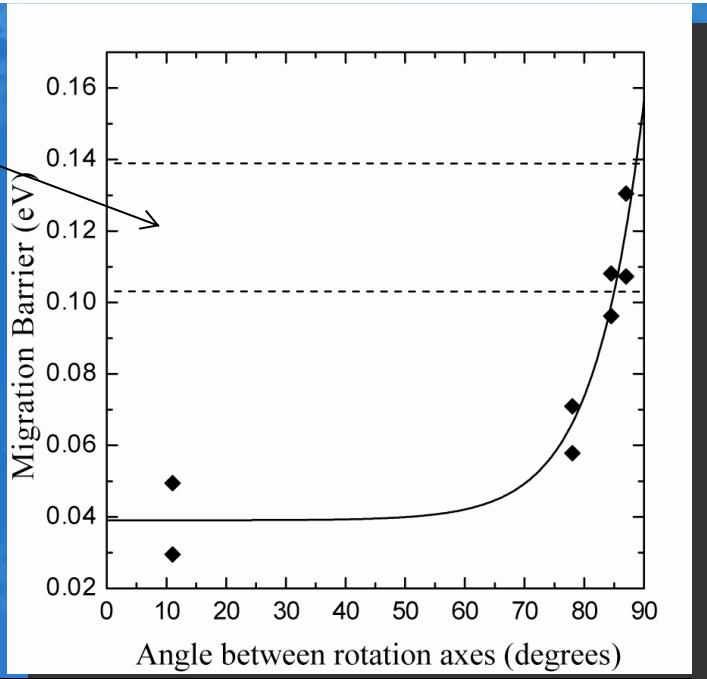
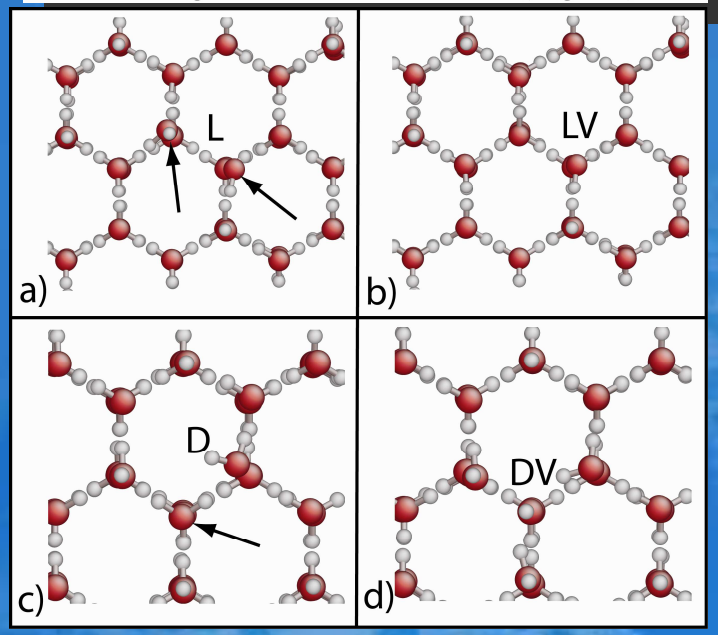
L-defect migration barriers (PRL **96,** (2006))



Results/Conclusions:

- Intrinsic D-defect migration barrier does not appear to be higher that of L-defect.
  - No intrinsic mobility issues, consistent with existence of traps.

- Both D and L defect strongly bind to vacancy, with essentially the same binding energy: ΔE=-0.55 eV:
  - Vacancy strong trapping center but affects D and L defects in similar fashion: may not explain observed D-activity.



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