Phosphate Aggregation:

Comparison of Polarizable and Non-Polarizable Force Fields

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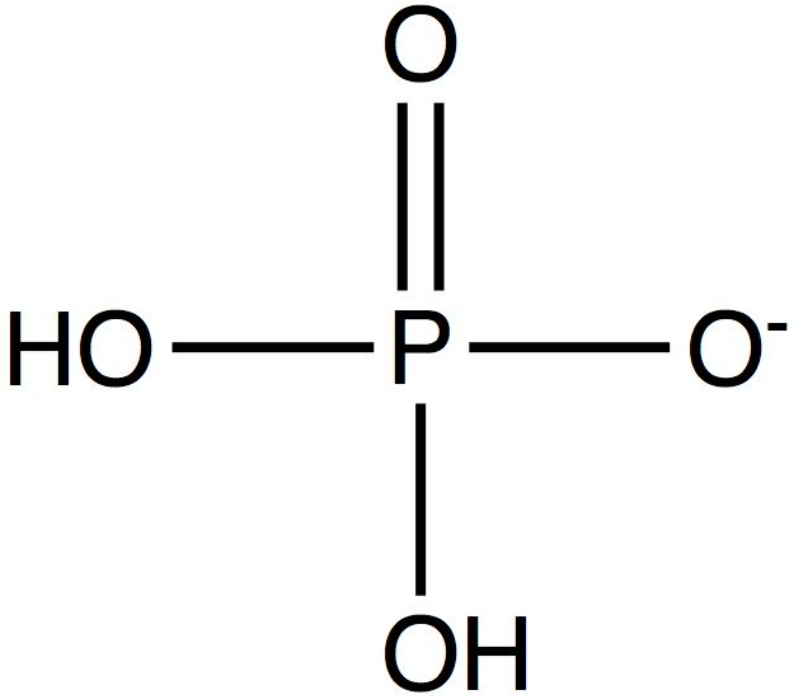
UNIVERSITY OF NOTRE DAME

The Goal

$H_2PO_4^-$

- It’s everywhere!



The Goal

$H_2PO_4^-$

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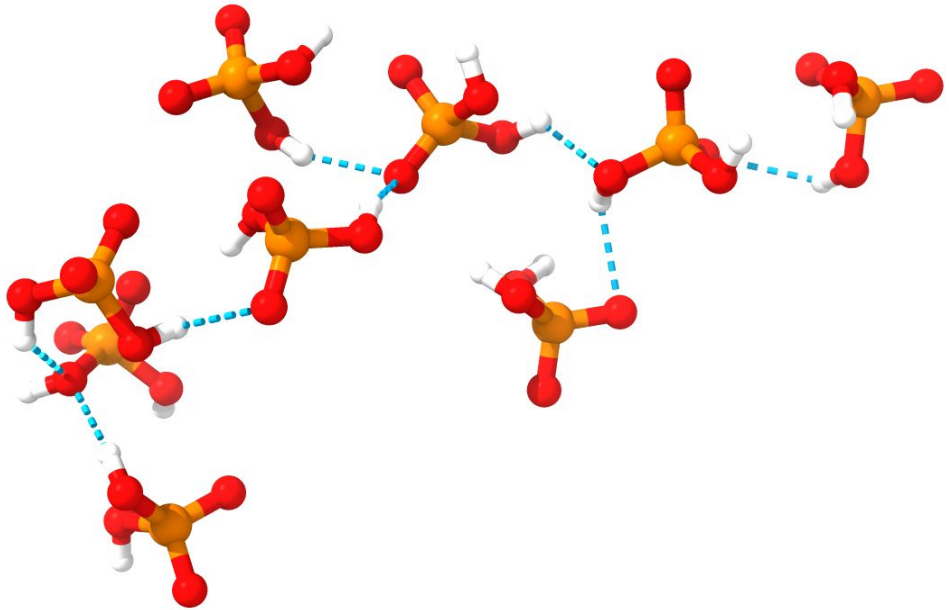


The Goal

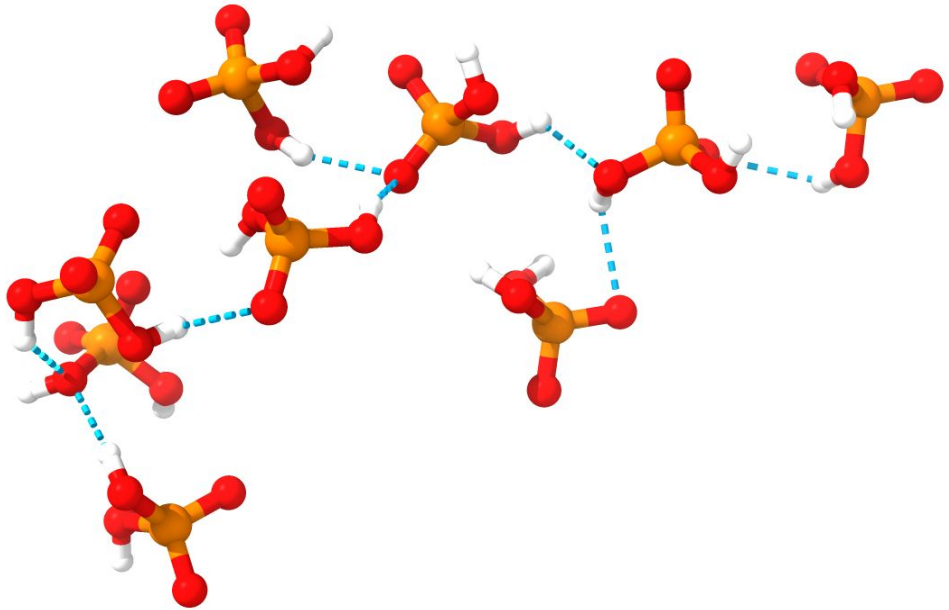
$H_2PO_4^-$

- It's everywhere!

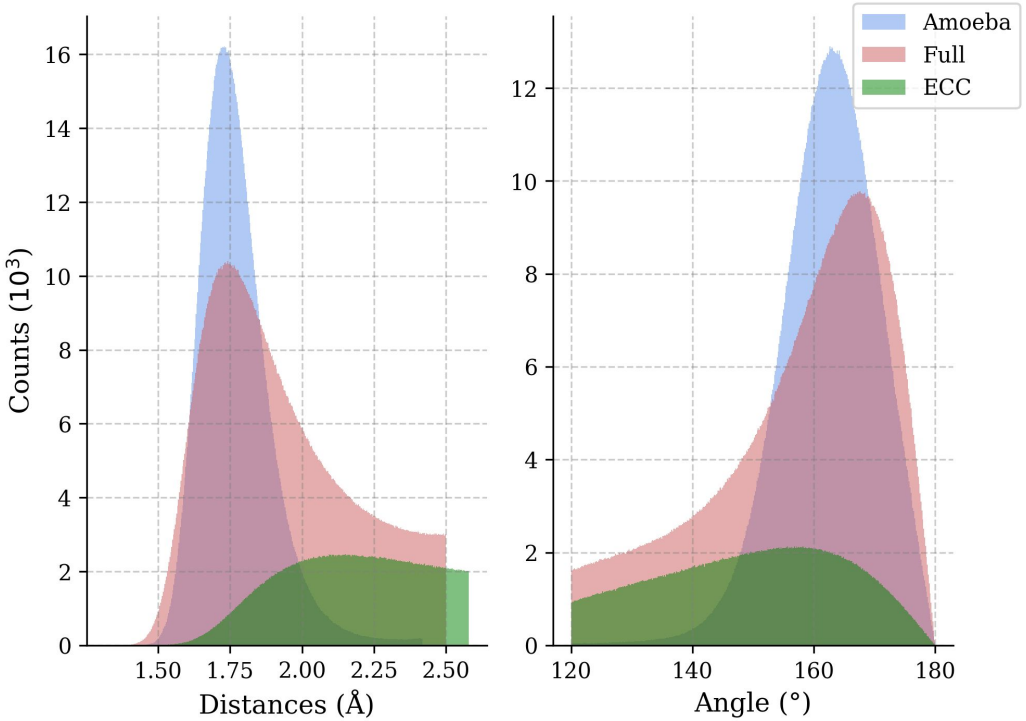
How does $H_2PO_4^-$ aggregate?

How do force field parameters affect aggregation?

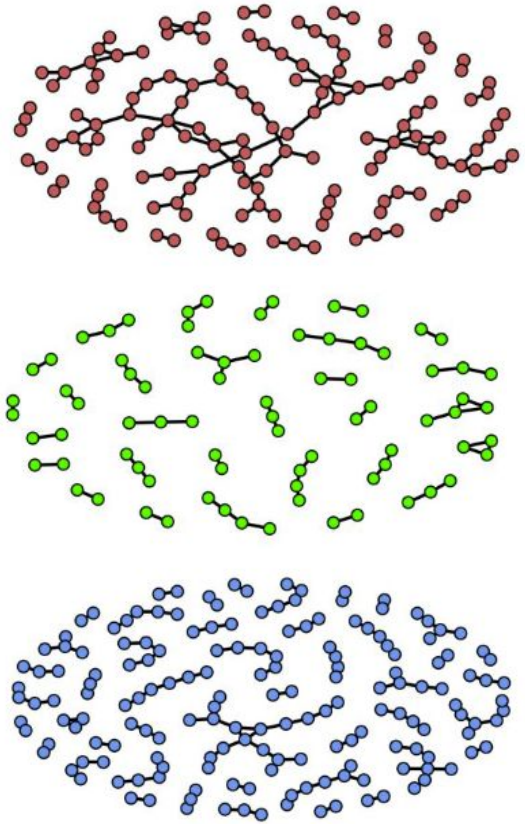
- *Full charge*
- *ECC (scaled charged)*
- *AMOEBA (polarization)*



Aggregate Structure



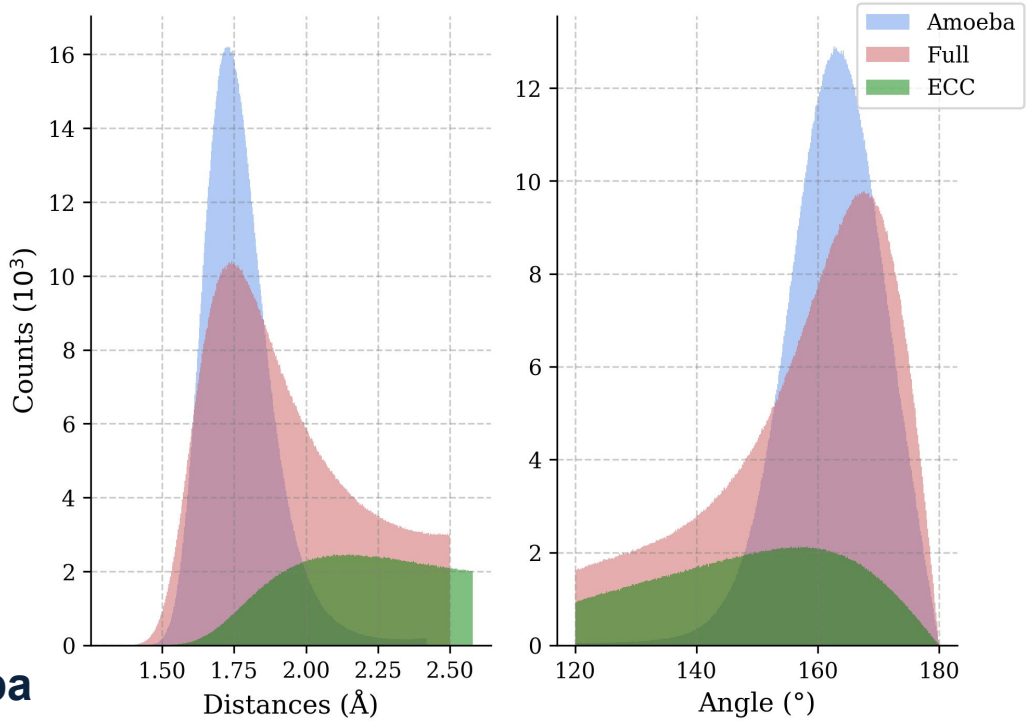
Aggregate Structure



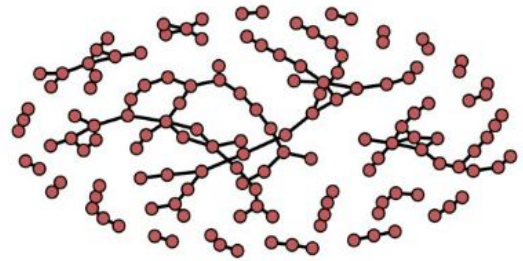
Full

ECC

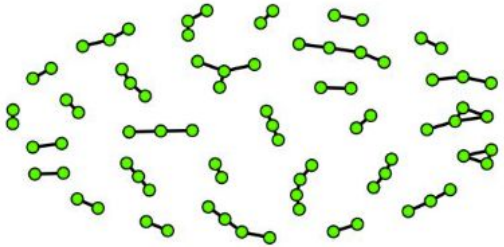
Amoeba



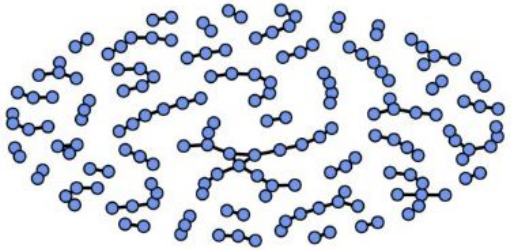
Aggregate Structure



Full



ECC



Amoeba

How does $H_2PO_4^-$ aggregate?

- *Chain-Like structures*
- *Random Network Topology*

How do force field parameters affect aggregation?

- *Largest impact at close range*
- *Macro structure consistent*

Acknowledgements

- Dr. Steven A. Corcelli
- Dr. Erin Brossard
- Nell Karpinski
- Shuang Wu
- Kaitlyn Handy
- Isabel Thompson

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