How to Assess AIMD Papers: a Guide for the Computational Potential of Zero Charge

Arthur Hagopian

May 27, 2025

Purpose of this Note

This short guide is written for colleagues in our research group who are primarily experimentalists. Its goal is to help you navigate and evaluate scientific papers that rely on **ab initio molecular dynamics (AIMD)** simulations, a method widely used in computational chemistry to model the atomic-scale behavior of systems in realistic (e.g., liquid, finite temperature) conditions. A specific focus is made towards the evaluation of the potential of zero charge (PZC).

Where to Look: The "Computational Details" Section

Most computational chemistry papers include a section called:

- **Computational Details**
- **Methods**
- **Theoretical Methods**

This section typically appears:

- Before the Introduction section
- At the end of the main text (before the Acknowledgements)
- In the Supporting Information (SI)

Key Elements to Look For

To evaluate whether a PZC evaluated from an AIMD study is trustworthy and of high quality, check for the following information (you can directly Ctrl+F the keywords written in **blue** in the following subsections for a faster research):

1. Software and Level of Theory

- Name of the **code**, **package** used (e.g., CP2K, VASP, Quantum ESPRESSO)
- Type of calculation: **AIMD** (Ab Initio Molecular Dynamics) should be clearly stated
- Exchange-correlation **functional**: e.g., PBE, RPBE, PBEsol, BLYP, SCAN (GGA functionals typically underestimate the WF/PZC by about 0.2 – 0.4 V)
- **Dispersion** corrections: DFT-D3, Grimme corrections, or van der Waals functionals (no dispersion corrections can lead to a stronger underestimation of the WF/PZC)

2. Simulation Parameters

- **Time step** for integration (typically 0.5–1.0 fs)
- **Simulation time** (at least several picoseconds, ideally more than 10 ps)
- **Thermostat** method: e.g., Nosé-Hoover, CSVR, Langevin

3. System Setup

- Size of the simulation **cell**: e.g., 3 x 4, 6 x 6 (a cell smaller than 6 x 6 can lead to an underestimation of the WF/PZC by about 0.2 – 0.6 V)
- Number of **atomic layers** (at least 4 layers)
- Length of the **water** region (should be > 20 Å, otherwise possible uncertainty on the PZC of about 0.3 V for the cSHE method)

4. Reference Potential Method

- The method **WF** or **cSHE** is always clearly stated
- Any PZC obtained via the WF method is hardly reliable due to the non-equilibration of the surface potential of water at the water/vacuum interface
- If the cSHE method has been used, consider a possible uncertainty of 0.15 – 0.25 V

Final Advice

- A good AIMD paper clearly states its approximations and limitations.
- Be cautious with very short simulations or small system sizes.
- If anything is unclear, feel free to reach out—I'm happy to help interpret the computational part of any paper.