The New Implicit Solvent Implementation in SIESTA

The Challenge:

Simulating every individual solvent molecule is computationally expensive, limiting simulations to small systems or short timeframes.

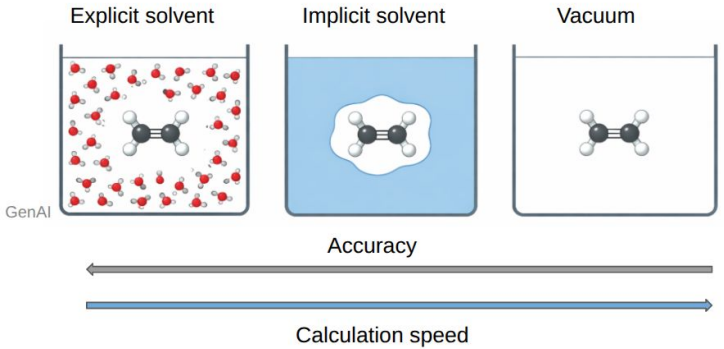
The Solution:

SIESTA's Rigid Cavity Implicit Solvent.

Available in **ASAP 2026.0**

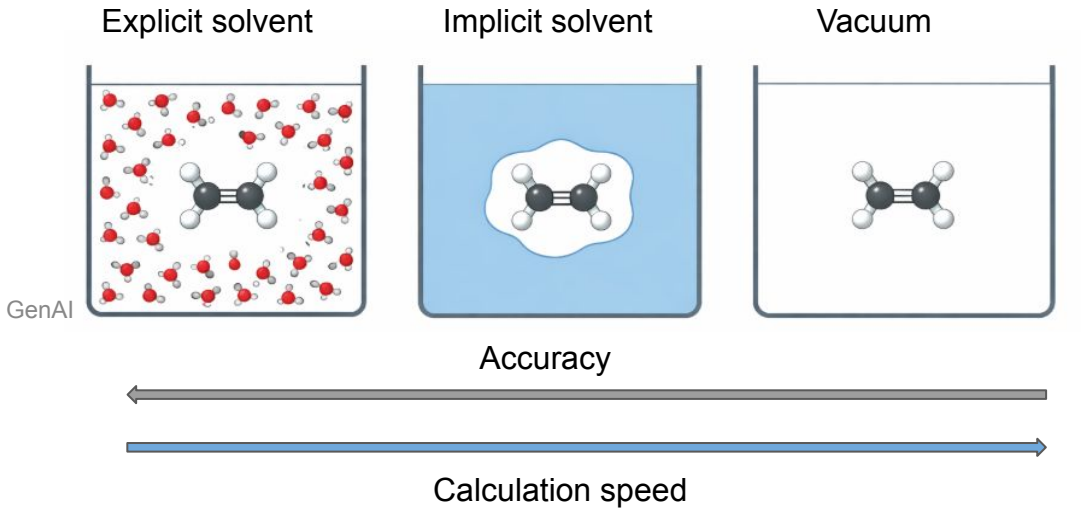
Strategic Impact:

- **Accelerated Long-Time Dynamics**
- **Thermodynamic Insights:** solvation free energies, stabilization of charged species…



Modelling Solvents in DFT

Traditional simulations involve modeling every individual solvent molecule, often resulting in prohibitive costs for large systems. **Implicit solvent model offers a strategic balance** between computational efficiency and accuracy.



Implicit Solvent Model

- The solvent is **treated as a continuous medium**, defined by bulk properties like its dielectric constant, rather than individual molecules.

- It effectively captures crucial solvation effects, such as the stabilization of charged species and the screening of electrostatic interactions, which are important for studying molecules and reactions in solution.

- When to use implicit solvent?
  - Interface & Surface Science; Surface Adsorption
  - High-Throughput Thermodynamics; Solvation Free Energies & Charged Systems
  - Large-Scale Structural Evolution: conformational Changes

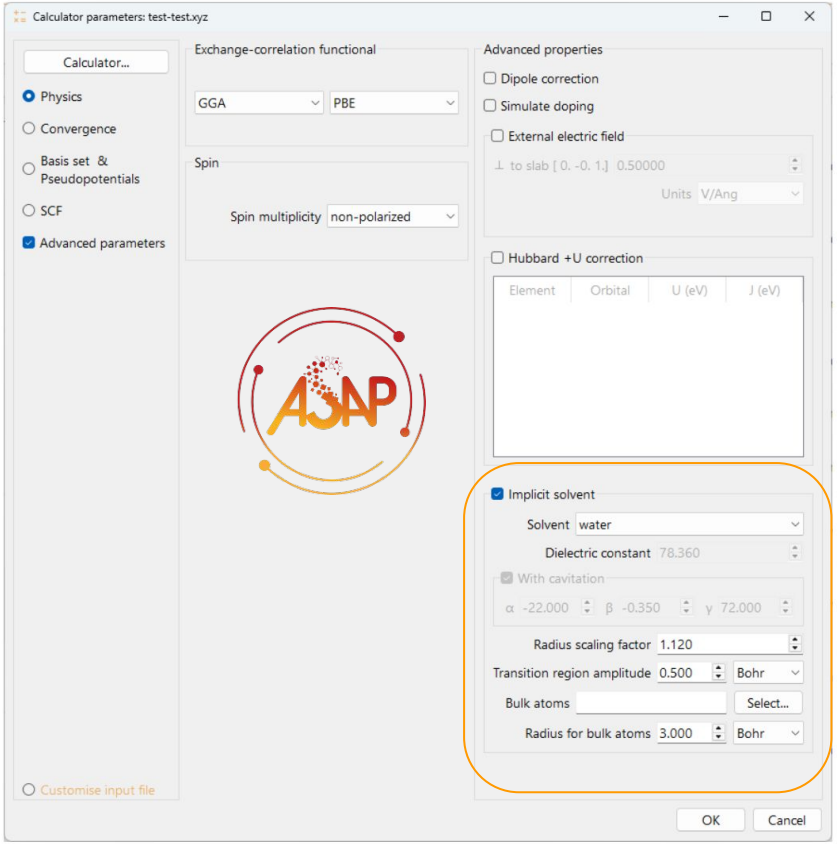
ASAP 2026.0: Launching Implicit solvent for SIESTA

ASAP provides a unified environment for both SIESTA and QE. **Implicit solvent** integration is exclusive to the **SIESTA solver.**

Rigid cavity model: core implementation directly within the SIESTA source code.

Funded by the European Union under the HORIZON-MSCA-2021 grant.

A functional preview version starting in **ASAP 2026.0**.

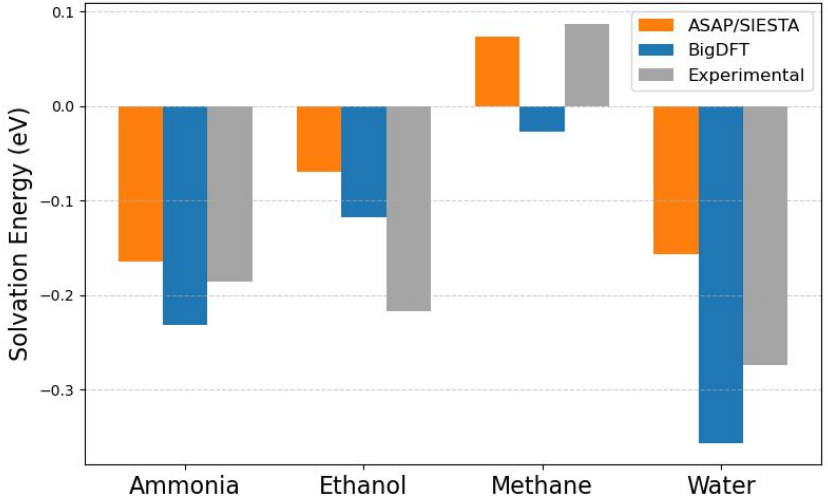


Validation of the implementation

ASAP/SIESTA successfully reproduces the solvation energy trends of the BigDFT reference.

The model shows consistent agreement with experimental data. MAE of 0.075eV.

Solvation results are highly sensitive to the defined cavity region. ASAP GUI default parameters provide a consistent physical baseline, though complex systems may require further radii optimization.



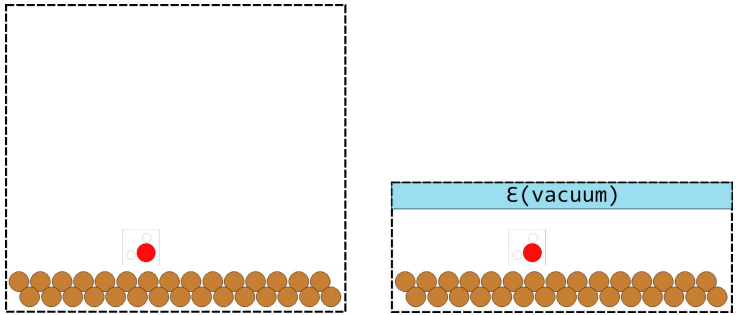
* ASAP 2026.0. SIESTA5.1 Mescutoff: 400Ry, Vacuum:12 Ang. Basis set: DZP. Cavity model: Radius scaling factor: 1.12, Δ: 0.5.
* BigDFT- J. Chem. Phys. 144, 014103 (2016): doi: 10.1063/1.4939125
*Experimental (MNSol) database- uncertainty ±0.009eV
https://comp.chem.umn.edu/sds/mnsol/mnsol.cgi

A Side-Effect: Enabling Non-Periodic Calculations

SIESTA no longer requires large vacuum boxes to avoid artificial periodicity. The new psolver, developed for the implicit solvent implementation, enables the calculation of electrostatic potential for various boundary conditions: bulk, surface, wire, and isolated systems.

SIESTA can now be used as a non-periodic or semi-periodic DFT code. The new feature automatically detects a system's periodicity and sets the appropriate boundary conditions.

This feature is particularly valuable for isolated systems (e.g., molecules, nanoclusters) as it eliminates the spurious long-range interactions from repeated periodic images.



Left: A large vacuum box is used to minimize interactions between periodic images.
Right: The new psolver automatically applies a free boundary condition

Next Steps: Start Your Atomistic Simulation

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