Topological data analysis of vortices in the magnetically-induced current density in LiH molecule - supporting information

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Quantum chemistry calculations

The experimental geometry of LiH molecule was used (R(Li-H) = 1.595 Å).[1] J^B and $\nabla \vec{J}^{B_\perp}$ tensors were calculated analytically in the development version of the DIRAC[2,3] software (commit hash `2330f11`) with the Dirac-Coulomb Hamiltonian, the B3LYP exchange-correlation functional,[4,5] and the def-TZVP[6] basis set applied for both atoms. London atomic orbitals[7–9] and the simple magnetic balance scheme[10] were applied in response calculations. The densities were exported on the cube grid of 128 points in each Cartesian direction using the default visualization options in DIRAC.

Description of included files

- The `coordinates` directory contains files with molecular geometry, including the file in `XYZ` format with the geometry in Å (useful for calculations) and the file in `CSV` format with the same geometry in a.u. (useful for visualization).
- The `data/LiH_MICD/dirac_data` directory contains:
  - the input files for DIRAC (`data/LiH_MICD/dirac_data/inputs`),
  - the outputs of calculations (`data/LiH_MICD/dirac_data/outputs`),
  - the files with the magnetically-induced current density tensor and its gradient exported on a 3D grid in text format (`data/LiH_MICD/dirac_data/plotfiles`)
- The `data/LiH_MICD/dirac_data/vti` directory contains files prepared for analysis in TTK in `VTI` format:
  - `start_data_omega_bz.vti` contains the $\Omega^{B_\perp}$ scalar field ("`omega_bz`") and the scalar field corresponding to the $\perp$-component of the curl of the $\vec{J}^{B_\perp}$ vector field (("`bz_wz`"));
  - `start_data_bz.vti` contains the $\vec{J}^{B_\perp}$ vector field, with its $x/y/z$-components referred to as "`bz_jx`", "`bz_jy`", "`bz_jz`", respectively;
  - `start_data_jb_tensor.vti` contains the elements of the full J^B tensor. Their names, "`b`α`_j`β", refer to the α-component of the magnetic field and the β-component of the current density vector.
- The `pvsm` directory contains a state file (in `PVSM` format) demonstrating the analysis in TTK. It reproduces the images included in the publication.

Description of the workflow

- DIRAC calculations are done in three steps, as discussed in the official DIRAC tutorial.

- TTK analysis can be reproduced with `paraview --state=pvsm/lih.pvsm`.

A detailed description of the data and the workflow is also available on a dedicated website (link in the official manuscript).

References

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