

Beyond Born-Oppenheimer Physics of Solids

Ville J. Härkönen

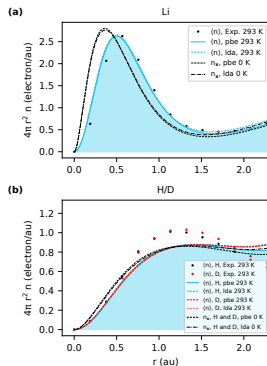
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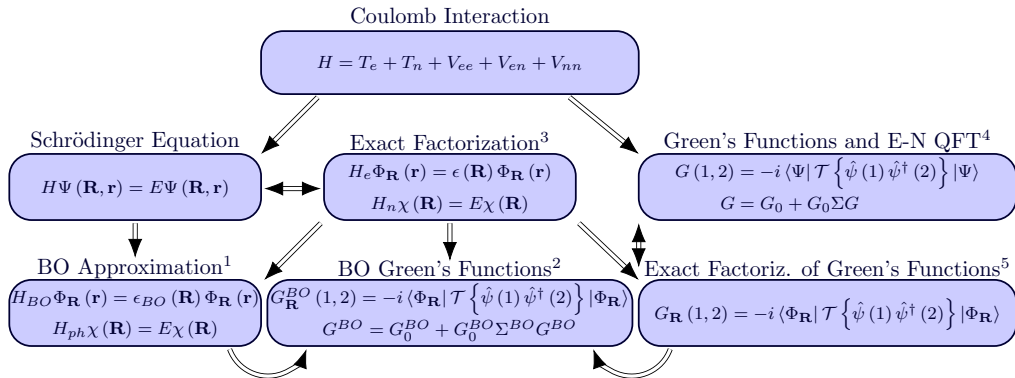
- **Doctoral researchers:** Gentrit Zenuni, 1-2 to be hired 8/2026; **Msc student** Emin Besic; **Bsc students:** Joonas Fält, Justus Korhonen.
- **Collaborators:** E. K. U. Gross (Hebrew University of Jerusalem), Patrick Rinke (Technical University of Munich), Ivan Gonoskov (Friedrich Schiller University Jena), Simo Huotari (Helsinki University, if measurements necessary), Matthew Krzystyniak (Vesuvio, neutron scattering experiments), Jouko Nieminen (in house).
- **Home page of the group:** <https://research.tuni.fi/mbt/>.

- Major success in the description of atoms, molecules, solids.
- Essentially always approximations for molecules and solids.
- Born-Oppenheimer approximation very central, always assumed for solids.

- Experiments suggest BO breakdown in LiH, no beyond-BO studies exist for solids, quantum mechanical nuclei within BO leave a discrepancy.
- High- T_c hydride superconductors show large **unexplained** gap in T_c between experiment and theory.
- Open question on the existence of solid hydrogen, solids of light elements in general.



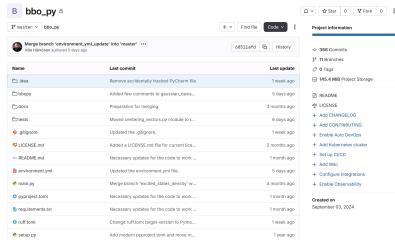
¹G Vidal-Valat et al. *Acta Crystallog. Sect. A* 48 (1992); V. J. Härkönen. *J. Phys.: Condens. Matter* 38.4 (2026), p. 045501; I. A. Troyan et al. *Advanced Materials* 33 (2021); V. J Härkönen. *arXiv:2311.06114 (in peer review, Reports on Progress in Physics)* (2023); E. Wigner and H. á. Huntington. *J. Chem. Phys.* 3 (1935), pp. 764–770; W. Nellis. *Phil. Mag. B* 79.4 (1999), pp. 655–661; J. M. McMahon et al. *Rev. Mod. Phys.* 84 (2012), pp. 1607–1653; J. M. McMahon. *Phys. Rev. B* 84 (2011), p. 220104; P. V. Hobbs. *Ice Physics*. OUP Oxford, 2010; A. Hermann, N. Ashcroft, and R. Hoffmann. *Proc. Nat. Acad. Sci.* 109.3 (2012), pp. 745–750



1. M. Born and R. Oppenheimer. *Ann. Phys. (Leipzig)* 389 (1927); K. Huang and M. Born. *Dynamical Theory of Crystal Lattices*. 1954.
2. E.K.U Gross, E. Runge and O. Heinonen, *Many-Particle Theory*. Adam Hilger, 1991.
3. G. Hunter. *Int. J. Quant. Chem.* 9 (1975); N. I. Gidopoulos and E. K. U. Gross. *Phil. Trans. R. Soc. London* 372 (2014).
R. Requist and E. K. U. Gross. *Phys. Rev. Lett.* 117 (2016); A. Abedi, N. T. Maitra, E. K. U. Gross *Phys. Rev. Lett.* 105 (2010).
4. G. Baym. *Ann. Phys. (NY)* 14 (1961); V. J. Härkönen, R. van Leeuwen, and E. K. U. Gross. *Phys. Rev. B* 101 (2020);
V. J. Härkönen *J. Phys. A: Math. Theor.* 57 (2024); V. J. Härkönen *J. Phys. A: Math. Theor.* 58 (2025);
V. J. Härkönen *arXiv:2604.11858* (2026).
5. V. J. Härkönen. *Phys. Rev. B* 106 (2022).

- Beyond Born-Oppenheimer Python (BboPy).
- Can systematically compute quantities like electron density and structure factors ab initio¹. Aim $G = G_0 + G_0 \Sigma G \dots$
- Will be made open source.

¹V. J. Härkönen. *J. Phys.: Condens. Matter* 38.4 (2026), p. 045501



The screenshot shows the GitHub repository for 'bbo_py' by Ville Härkönen. It displays the commit history, project information, and a list of files.

Name	Last commit	Last update
main	Remove accidentally tracked PyCharm file	1 week ago
CONTRIBUTING	Added few comments to generate_utils...	5 days ago
docs	Preparation for merging	3 months ago
tests	Moved centering_vectors.py module to L...	6 days ago
gpgnome	Updated the gpgnome	1 week ago
LICENSE.md	Added a LICENSE.md file for current lic...	2 months ago
README.md	Necessary updates for the code to work ...	1 month ago
environment.yml	Updated the environment and file	5 days ago
main.py	Merge branch 'removed_state_density' w...	4 months ago
pyproject.toml	Necessary updates for the code to work ...	1 month ago
requirements.txt	Necessary updates for the code to work ...	1 month ago
utils.py	Change ruftools target version to Pytho...	1 week ago
setup.py	Add modern pyproject.toml and move in...	1 year ago

Project information

- 368 Commits
- 11 Branches
- 4 Tags
- 145.4 MB Project Storage
- README
- LICENSE
- CONTRIBUTING
- Enable Auto DevOps
- Add Ruleset (viewer)
- Set up CI/CD
- Add files
- Configure integrations
- Enable Observability
- Created on September 23, 2024

- **Objective 1:** Study of beyond-BO electron density (WP1, planned 1/2026-12/2027)². BboPy development going well, some set backs. Aleksi Hartikainen won the FPS Master's Thesis Prize 2025.
- **Objective 2:** First beyond-BO electronic G and band structures (WP2, planned 7/2026-7/2028). Promising. Depends on Objective 1.
- **Objective 3:** First beyond-BO theory of superconductivity and its implementation (WP3, planned 1/2026-). Depends on Objectives 1 and 2.
- **Objective 4:** Development of (Pauli–Fierz³) QFT/GFT^{4,5} with photons (WP4, planned 1/2027-). Head start.
- **Objective 5:** Use of our theoretical tools to study gravity^{5,6} (WP5, planned 7/2027-). Head start.

²V. J. Härkönen. *arXiv:2311.06114 (in peer review, Reports on Progress in Physics)* (2023);

V. J. Härkönen. *J. Phys.: Condens. Matter* 38.4 (2026), p. 045501

³M. Ruggenthaler, D. Sidler, and A. Rubio. *Chem. Rev.* 123.19 (2023), pp. 11191–11229

⁴V. J. Härkönen. *J. Phys. A: Math. Theor.* 57.46 (2024), p. 465402

⁵V. J. Härkönen. *arXiv:2604.11858* (2026)

⁶V. J. Härkönen. *J. Phys.: Conference Series*. Vol. 3017. 1. 2025, p. 012023

Thank You!