

Philip Hoggan, born 15.3. 1961 in Aberystwyth, GB.

Married, two children.

Admitted to Trinity College after entrance examination, Cambridge 1978

Graduated Master of Chemistry 1983 (and Master of Wine) from Cambridge.

DSc (higher doctorate by research), Nancy, France 1991.

Appointed lecturer at Caen University in 1992. Research in the Catalysis laboratory:

Theme: combining theory and FTIR of reaction intermediates.

Professor and chair of Theoretical Chemistry, Clermont 1998 to present. Current research: Quantum Monte Carlo for molecules on solid surfaces, DFT and AIMD for processes at III-V semi-conductor interfaces. CNRS (National Research Council) leave for research: full-time 2016-2017, part (half) time 2017-2019.

About 80 peer-reviewed publications (h=19 over 1100 citations). Editor and referee of several journals.

Organised several international conferences: e.g. Quantum Systems in Chemistry and Physics 15 in Cambridge (2010). Record attendance (137 from 5 continents).

A D Buckingham 80th birthday session. Edited and published 650pp proceedings.

Also Molecular Electronic Structure (MES) MEST (2012) MES14, MESBA (2016) and MES 2018 (Metz) International workshops.

French representative of International Society for Theoretical Chemical Physics 2002- present.

2013-2014: PRACE Award: 6 million core hours on JUQUEEN. PRACE Call 7 Panel: Chemistry and Materials expert.

ERC Advanced Grant as collaborator of QMC consultant for Geert-Jan Kroes 2014-2017 (Leiden Institute of Chemistry, NL). Post-doc in this context: Katharina Doblhoff-Dier 2015-2016 (now Assistant Professor in Leiden).

Editor, Advances in Quantum Chemistry: vol 67 (published December 2013) vol 68 (published January 2014). Total 627pp. Vol 76 2018.

Post doc. Regional fund, with FEDER support: CPER 2013: Ali Bagci (18 months 2013-2015)

Correspondent for IP in GDR CORREL.

Vice-president of Beaudonnat school council (Aubière, France).

Bibliometric values: h=19 1100 citations (1 nov 2019).

PUBLICATIONS IN INTERNATIONAL Peer-Reviewed Journals 2014 to present.

- 1 Chapter 3 - Asymptotic Expansions of Barnett–Coulson–Löwdin Functions of High Order
Adv. Quantum Chem. 68 (2014) *Pages 43-76* A. Sidi, D. Pinchon, P.E. Hoggan
- 2 Chapter 5 - Relative Advantages of Quantum Monte Carlo Simulation for Changing Electron Correlation: CO Reactions on Copper and Platinum Catalysts Adv. Quantum Chem. 68 (2014) *Pages 89-103* P.E. Hoggan, A. Bouferguene
- 3 Chapter 9 - A Density Functional Theory Study of the Adsorption of 2-Cyclohexenone on Rh(111) Adv. Quantum Chem. 68 (2014) *Pages 175-190*, R. Ghomari, A. Bouferguene, P.E. Hoggan, S.M. Mekelleche
- 4 Performance of numerical approximation on the calculation of overlap integrals with noninteger n-Slater orbitals, Phys. Rev. E., 89 5 (2014) 053307. A. Bağcı and P. E. Hoggan
- 5 PHYSICAL REVIEW E 91, 023303 (2015). Benchmark values for molecular two-electron integrals arising from the Dirac equation, A. Bağcı and P. E. Hoggan
- 6 Vapor liquid solid-hydride vapor phase epitaxy (VLS-HVPE) growth of ultra-long defect-free GaAs nanowires: Ab initio simulations supporting center nucleation
The Journal of Chemical Physics 140, 2014, 194706 Y André, K Lekhal, P. Hoggan, G. Avit, F. Cadiz, A. Rowe, D. Paget, E. Petit, C. Leroux, A. Trassoudaine, M. Reda Ramdani, G. Monier, D. Colas, R. Ajib, D. Castelluci and E. Gil.
- 7 Quantum Monte Carlo for Activated Reactions at Solid Surfaces: Time Well Spent on Stretched Bonds, Philip E. Hoggan* and Ahmed Bouferguene, International Journal of Quantum Chemistry, 2014,114 p1150–1156
- 8 ANDRE Y., TRASSOUDAINE A., AVIT G., LEKHAL K., RAMDANI M., LEROUX C., MONIER G., VARENNE C., HOGGAN P., CASTELLUCI D., BOUGEROL C., REVERET F., LEYMARIE J., PETIT E., DUBROVSKII V., GIL E.
Hydride VPE: the unexpected process for fast growth of GaAs and GaN nanowires with record aspect ratio and polytypism-free crystalline structure SPIE 8923 vol. 1, 8923-23, 2014
- 9 Benchmark values for molecular three-center integrals arising in the Dirac equation. A. Bağcı and P. E. Hoggan. Phys. Rev. E 92, (2015) 043301
- 10 An Application of the Gaussian Transform for Approximating Some Bessel Functions and Multicenter Integrals Involving 1s Slater-Type Orbitals, Adv. Quantum Chem. 73 (2016) ch 6, Pages 139-144, Philip E. Hoggan, Jorge E. Perez, Ahmed Bouferguene
- 11 Diffusion Monte Carlo for accurate dissociation energies of 3d transition metal containing molecules
Katharina Doblhoff-Dier, Joerg Meyer, Philip E. Hoggan, Geert-Jan Kroes, and Lucas K Wagner. J. Chem. Theory Comput. 2016, 12, 2583–2597.
Publication Date (Web): May 13, 2016 (Article) DOI: 10.1021/acs.jctc.6b00160

12 Mediterranean Journal of Chemistry, Theory and simulation of selective hydrocarbon oxidation at copper surfaces: Part I methane mild oxidation to methanol, formaldehyde and formic acid

Noureddine Absi and Philip E. Hoggan, MES14 Proc. p33-40 2015

13 Mediterranean Journal of Chemistry, Theory and simulation of selective hydrocarbon oxidation at copper surfaces:

Part II short-chain alkene epoxidation and bi-reactions.

Noureddine Absi and Philip E. Hoggan, MES14 Proc. P41-45 2015

14 Solution of the Dirac equation using the Rayleigh-Ritz method: Flexible basis coupling large and small components. Results for one-electron systems

A. Bağcı and P. E. Hoggan

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15 Quantum Monte Carlo investigation of two catalytic reaction paths for hydrogen synthesis on Pt(111). Noureddine Absi and Philip E. Hoggan in Recent progress in Quantum Monte Carlo, ed. S.Tanaka, L. Mitas, P-O Roy, ASC books, Symposium Series (Pacifichem) (2016). Chapter 5, pp 77–88

16 Scaling analysis of Self-assembled structures and related morphological information in epitaxial growth, S. Blel, A. B.H. Hammouda, B. Mahjoub, P. E. Hoggan and B. Oujia, Superlattices and Microstructures · 102, 155-165 (2017).

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17 Quantum Monte Carlo Calculations on a Benchmark Molecule–Metal Surface Reaction: H₂ + Cu(111), Katharina Doblhoff-Dier, Joerg Meyer, Philip E. Hoggan and Geert-Jan Kroes, J. Chem. Theory Comput., 2017, 13 (7), pp 3208–3219

18 Local NMR susceptibility and nuclear shielding tensors. N. Joudieh, A. Bağcı and P. E. Hoggan, Advances in Quantum Chemistry, **76** (2018) p169-183.

19 Combined angle-resolved X-ray photoelectron spectroscopy, density functional theory and kinetic study of nitridation of gallium arsenide

H. Mehdi ¹, G. Monier ^{1,*}, P. E. Hoggan ¹, L. Bideux ¹, C. Robert-Goumet ¹, V. G. Dubrovskii ^{2,3,4}

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In Applied Surface Science <https://doi.org/10.1016/j.apsusc.2017.08.002>

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20 Quantum Monte Carlo Calculations for Industrial Catalysts: Accurately Evaluating the H₂ Dissociation Reaction Barrier on Pt(111) . Philip E. Hoggan, *Advances in Quantum Chemistry*, **76** (2018) p273-280.

21 Analytical evaluation of relativistic molecular integrals. I. Auxiliary functions, A Bagci and P. E. Hoggan, *Rend. Fis. Acc. Lincei* **29** (2018) p191-199. <https://doi.org/10.1007/s12210-018-0669-8>

22 Quantum Monte Carlo activation barrier for hydrogen dissociation on copper to unprecedented accuracy. Philip E Hoggan,

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23 DFT and experimental FTIR investigations of early stages of GaAs (100) and (111)B surface nitridation, Guillaume Monier, Philip E Hoggan, Christine Robert-Goumet, Luc Bideux, Daniel Paget, Paul Dumas, Stephan Kubsky, *J. Appl. Phys* (Accepted)

24 Analytical evaluation of relativistic molecular integrals. I. Auxiliary functions, A Bagci and P. E. Hoggan, *Rend. Fis. Acc. Lincei* **29** (2018) p191-199. <https://doi.org/10.1007/s12210-018-0669-8>

25. Quantum Monte Carlo activation barrier for hydrogen dissociation on copper to unprecedented accuracy. Philip E Hoggan,

[arXiv:1511.07857](https://arxiv.org/abs/1511.07857) [**cond-mat.mtrl-sci**] (Submitted on 24 Nov 2015)

26. Analytical evaluation of relativistic molecular integrals. II. Computational aspect for relativistic molecular auxiliary functions. Ali Bagci, Philip Eric Hoggan and Muzaffer Adak, *Rend. Fis. Acc. Lincei* LYNC-D-18-00128R1 revision submitted 26.07.2018 online 18 aug 2018.

27. Physisorption energy of H and H₂ on clean Pt(111) as a useful surface energy reference in Quantum Monte Carlo calculation, Rajesh O. Sharma and Philip E. Hoggan, *Advances in quantum chemistry* **79** (2019) p311-322

28. Considering a mixed atomic basis set composed of only 1s STO and 1s GTO in molecular calculations J.E. Pérez^{1*}, J.C. Cesco², C.J. Alturria Lanzardo³, D.G. Zaccari¹, F.S. Ortiz¹, A.T. Soltermann⁴, P. E. Hoggan, *Chemistry Research Journal*, 2019, 4(1):60-66