

# Curriculum Vitae

Katalin Gaál-Nagy



## Personal data

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## Studies and Research activities

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10/94 – 05/99	Study of physics at the Universität Regensburg, Germany
05/99	<i>Diplom</i> in physics at the Universität Regensburg, Germany final degree of 1.32 <sup>1</sup>
12/99	<i>Erstes Staatsexamen für das Lehramt an Gymnasien</i> , final degree of 2.55 <sup>1</sup>
04/00 – 06/04	PhD student at the institute of theoretical physics, Universität Regensburg, Germany (supervisor: Prof. D. Strauch)
06/04	PhD degree with “Magna cum Laude” (very good)
02/04 – 08/08	Postdoc within the Nanoquanta Network of Excellence at the physics department, University of Milan, Italy

## Grants

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10/00 – 09/03	Fellowship founded by the Heinrich Böll Stiftung Germany, including research funds for attending international conferences.
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## Invited Seminars

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31/05/07	Università degli Studi di Milano-Bicocca (Italy)
13/06/07	SISSA, Trieste (Italy)
18/06/07	DEMOCRITOS, Trieste (Italy)
04/03/10	Oxford University/Trinity College, Oxford (United Kingdom)

## Collaborations

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06/07 – 12/07	Visiting scientist at the physics department Università di Roma “Tor Vergata”, collaboration with Prof. Rodolfo del Sole and Dr. Olivia Pulci
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<sup>1</sup>degrees from 1 (very good) to 6 (very bad)

## Attended workshops and conferences with contribution

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03/1998	Frühjahrstagung der Deutschen Physikalischen Gesellschaft (Regensburg, Germany)
03/2000	Frühjahrstagung der Deutschen Physikalischen Gesellschaft (Regensburg, Germany)
09/2000	X Workshop on Computational Materials Science (Villasimius, Sardinia, Italy)
01/2001	X International Workshop on Computational Material Science: Total energy and force methods (Trieste, Italy)
03/2001	Frühjahrstagung der Deutschen Physikalischen Gesellschaft (Hamburg, Germany)
09/2001	XI Workshop on Computational Materials Science (Villasimius, Sardinia, Italy)
03/2002	Frühjahrstagung der Deutschen Physikalischen Gesellschaft (Regensburg, Germany)
09/2002	XII Workshop on Computational Materials Science (Villasimius, Sardinia, Italy)
01/2003	XI International Workshop on Computational Material Science: Total energy and force methods Winter college on Numerical Methods in Electronic Structure Theory (Trieste, Italy)
03/2003	Frühjahrstagung der Deutschen Physikalischen Gesellschaft (Dresden, Germany)
09/2003	10th International Conference on Applications of Density Functional Theory in Chemistry and Physics (Brussels, Belgium)
09/2003	XIII Workshop on Computational Materials Science (Geremeas, Sardinia, Italy)
03/2004	Frühjahrstagung der Deutschen Physikalischen Gesellschaft (Regensburg, Germany)
01/2005	XII International Workshop on Computational Material Science: Total energy and force methods (Trieste, Italy)
05/2005	Nanoquanta Young Researchers' Meeting (Berlin, Germany)
09/2005	The 2005 Nanoquanta Workshop: 40 Years of the GW Approximation for the Electronic Self-Energy: Achievements and Challenges (Bad Honnef, Germany)
03/2006	Frühjahrstagung der Deutschen Physikalischen Gesellschaft (Dresden, Germany)
05/2006	Nanoquanta Young Researchers' Meeting (Rom, Italy)

## Attended workshops and conferences with contribution (continue)

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07/2006	The Epioptics-9: International School of Solid-State Physics (Erice, Italy)
09/2006	The 2006 Nanoquanta Workshop (Houffalize, Belgium)
01/2007	XIII International Workshop on Computational Material Science: Total energy and force methods (Trieste, Italy)
05/2007	Nanoquanta Young Researchers' Meeting (San Sebastian, Spain)
07/2007	40th Workshop of Solid State Physics on "Vibrations at surfaces - 12"
	42th Workshop of Solid State Physics on "Low Dimensional Dynamical Phenomena and Simulations" (Erice, Italy)
09/2007	12th Nanoquanta Workshop on Electronic Excitations. Time-Dependent Density-Functional Theory: advances and prospects (Aussois, France)
02/2008	CECAM tutorial "Basic techniques and tools for development and maintenance of atomic-scale software (Lyon, France)
05/2008	Nanoquanta Young Researchers' Meeting (Modena, Italy)

## Supervised graduations

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07/05 – 10/05	Tight-Binding calculations of Silicon Bands, Eugenio Cinquanta, <i>tesi triennale</i> (bachelor thesis)
06/06 – 10/06	Ab initio calculations of phonons for small Si nanocrystals Giulia Canevari, <i>tesi triennale</i> (bachelor thesis)
01/08 – 10/08	Ab-initio calculation of optical properties using a real-space slicing technique Carlo Motta, <i>tesi magistrale</i> (master thesis)

## Research-related activities

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09/97 – today	Member of the Deutsche Physikalische Gesellschaft
11/03	Participation at an experiment at the ILL in Grenoble
06/05 – today	Member of the Nanoquanta Network of Excellence
10/04 – today	Referee of various Journals

## Research topics

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- **High-pressure phase transitions in Si and Ge from ab initio methods**

In this field I work in particular on the phase transitions between the cd,  $\beta$ -tin, *Imma*, and sh phases of Silicon and Germanium using ab initio methods utilizing the plane-wave based codes QUANTUM-ESPRESSO and VASP. Here, the transition pressures have been obtained for hydrostatic conditions using various methods for determining the pressure, e.g., using an empirical equation of state or analyzing the stress tensor. From the components of the stress tensor, a method for investigating the phase transitions under non-hydrostatic conditions and the corresponding enthalpy barriers has been developed. Furthermore, the temperature dependence of the transition pressures has been investigated within the quasi-harmonic approximation. For this purpose, the phonon frequencies have been calculated for all phases at various values of the volume within and outside the stability range of the phase, which yields also to an investigation of soft phonon modes, polarization of the modes, Grüneisen parameters, etc. At the present I investigate the temperature dependence of the  $\beta$ -tin $\rightarrow$ *Imma* $\rightarrow$ sh transition within a fully quasi-harmonic treatment of the thermodynamic quantities, where also the temperature dependence of the pressure and the volume will be taken into account. Since these quantities depend strongly on the low-frequency phonon modes, these modes have to be calculated very accurately. For this purpose, a method to obtain convergence of phonon dispersion curves faster than usually based on a modification of the Fourier Interpolation procedure has been developed. Inspecting the origin (numerical vs. physical) of apparent soft phonon modes, a Kohn anomaly has been found for the bct structure beyond the stability range of the  $\beta$ -tin phase. A more detailed description can be found in the publications [1]-[8], and [13]. Some further projects are planned [25], [28], and [29].

- **Optical properties of the Si(113) surface from ab initio methods**

The optical properties of high-index Silicon surfaces have been studied within the independent particle approximation at the example system Si(113) $3\times 2$ ADI. The scope of this study is the calculation of a predictive reflectance anisotropy spectra (RAS), which reflects the features of the surface. Therefore, the electronic band structure, the imaginary part of the dielectric function, and the RAS have been investigated, where the surface relevant peaks of the RAS have been identified and mapped to the surface bands, which we discriminated from the projected bulk bands [10]. During this project, also methods for accelerating convergence tests have been developed and the TOSCA package (which has been developed for the ETSF) has been improved [11]. A possible continuation of this project will contain some ab-initio calculations of further surface reconstructions of Si(113) or tight-binding

investigations.

- **Analysis of phonons of oxidized Si clusters**

Since Silicon nanostructures play an important role in micro electronics, investigations in this direction will be performed. A first step was the investigation of the electronic properties [12]. In order to determine the temperature effects, the analysis of the phonons of oxidized Silicon nanocrystals of various size with ab initio methods using the code ABINIT has been performed [14]. Herewith, also an investigation of the influence of the spin has been performed [26]. A further project could be the investigation of silicon nanowires and nanotubes with a large diameter using density-functional methods with periodic boundary conditions.

- **Reflectance anisotropy spectra of oxidized Si(001)**

In this project the evaluation of various surface reconstructions during the oxidation process has been investigated using ABINIT and TOSCA. The reflectance anisotropy spectra for various surface constructions have been combined and compared with measured spectra which have been performed for various oxygen coverages. From the combined theoretical data, also surface differential reflectivity spectra have been calculated and compared with the experimental ones. Both, experimental and theoretical results, yield to an explanation of the kinetics of the oxygen adsorption [15][17].

- **Optical and vibrational properties of 3-tert-butyl-cyclohexene**

3-tert-butyl-cyclohexene is a molecule of biological and pharmaceutical interest. There exist two conformers and with respect to them various chemical reactions can occur. Because of this, it would be interesting to know, if these conformers can be distinguished by their vibrational and optical spectra. For this reason, the absorption spectra of 3-tert-butyl-cyclohexene have been calculated within standard density-functional methods at the independent-particle level using the QUANTUM-ESPRESSO package and within time-dependent density-functional theory using both, the Casida formalism and the real-time density-evolution method using the OCTOPUS package [19]. A shift of the oscillator strength to higher energies in the time-dependent density-functional spectra with respect to the independent particle ones has been found. The differences in the spectra of the two conformers have been traced back to the different buckling in the cyclohexene rings of the two conformers. Till now, only a measurement of the optical rotation exists, which might be investigated also. Here, it is necessary to implement the corresponding formula in the QUANTUM-ESPRESSO package. Afterwards, an implementation at the GW level is planned. Besides, a detailed analysis of the real part of the dielectric function starting from the results of the imaginary part [27] is in progress.

Concerning the vibrational properties, density-functional perturbation theory calculations using QUANTUM-ESPRESSO have been performed in order to obtain

the vibrational density of states. The two conformers could be distinguished by their frequency spectra, if the relevant features can be resolved in the experiments. Furthermore, an analysis of the eigendisplacements of the modes leads some conclusions with respect to the relative stability of the two conformers to each other and it was possible to identify the characteristic modes of this molecule [21].

- **Structural stability of the Si(331) surface**

In collaboration of an experimental group the reconstruction the vicinal Si(331) surface has been investigated. Comparing experimental STM measurements with the results of ab-initio calculations for various surface reconstructions it was possible to determine the surface reconstruction [18]. This study is based on various considerations about possible surface reconstruction elements [16] and a systematic test of the ones which are relevant for the Si(331) surface [20]. Furthermore, an analysis of the electronic structure, again combining experimental investigations with first-principle ones, has been performed [24]. Based on our results, a detailed investigation of the surface-resolved electronic band structure can give additional information.

- **Optical properties of polyynes and cumulenes**

Carbon-based materials possess many potential ability for future technologies. The formation of carbon chains (polyynes and cumulenes) is expected in the initial stage of small carbon cluster formation, on the road towards the fullerene structure. Carbon chains are also interesting systems because they can be found to connect different graphene fragments, and so they can play a crucial role in the charge transfer effects. For this reason a first-principle investigations of polyyne and cumulene prototypes has been performed in order to figure out characteristic features in their absorption spectra which can help to distinguish various isomers by optical measurements. Considering the spectra obtained within the density-functional theory employing the independent-particle approximation (DFT-IPA), the six prototypes can be distinguished by absorption measurements. Furthermore, since the DFT-IPA results are not always reliable for isolated systems, a general scheme to determine the prototype kind within optical spectra has been developed, which bases on common features of the DFT-IPA spectra and random-phase approximation results including the local-field effect [22].

- **Implementation of the optical matrixelements to the open-source package ABINIT**

The calculation of the optical matrixelements (with and without real-space cutoff) in independent-particle approximation based on ingredients resulting from density-functional theory calculations has been implemented to the open-source package ABINIT where also the correction from the non-local pseudopotential contribution has been added to this implementation [23].

## Additional and coordination activities

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03/01	Co-organizer of the <i>Frühjahrstagung der Deutschen Physikalischen Gesellschaft</i> in Regensburg (Germany)
04/00 – 09/00	Women's' representative of the physics department of the Universität Regensburg, member with voting power in the <i>Fachbereichsrat</i> (department committee) and advising member of various <i>Berufungskommissionen</i> (committee for filling chair positions at the physics department of the Universität Regensburg).
07/01 – 01/02	Associate of the women office
08/01	Participation at a workshop "Conflict management"
10/01 – 09/03	Elected representative of the Heinrich-Böll fellows of the region Germany-South
	Active member of the council of the Heinrich-Böll fellows
02/02 – 10/03	Active assistant of the green students party
10/02 – 10/03	Elected member of the students parliament
06/04 – 08/08	Local editor of the Nanoquanta Newsletter
06/06 – 08/08	Nanoquanta Young Researchers' Representative of the Milan Node
02/07 – 08/08	Elected representative of the research fellows in the council of the Physics Department of the University of Milan

## Teaching activity

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04/00 – 03/03 and 10/03 – 01/04	Preparation course for the examination in experimental physics (writing form) for the <i>Erstes Staatsexamen für das Lehramt an Gymnasium</i>
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## Computational experience

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- Programming: FORTRAN, IDL, C (basics), C++ (basics), csh scripts
- Experiences with big program packages (partially based on ab-initio methods): VASP, QUANTUM-ESPRESSO, ABINIT, GAUSSIAN, CP, OCTOPUS
- Experience with visualization programs: Molden, Xcrysden, gimp, IslandDraw
- Experience with word processing programs: Word, PowerPoint, Latex, OpenOffice
- Experience with web application programming: ABSolution, Java

## Languages

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- German (mother tongue)
- English (fluid)
- Italian (fluid)

## References letters can be requested from:

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- Prof. Dieter Strauch,  
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- Prof. Giovanni Onida,  
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- Prof. Rodolfo del Sole,  
CNR-INFN, and Dipartimento di Fisica,  
Università di Roma “Tor Vergata”,  
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- Dr. Pasquale Pavone,  
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## References

- [1] **Temperature and Dynamical Effects on the High-Pressure Cubic-Diamond  $\leftrightarrow$   $\beta$ -Tin Phase transition in Si and Ge**, K. Gaál-Nagy, A. Bauer, M. Schmitt, K. Karch, P. Pavone, and D. Strauch, Phys. Stat. Sol. (b) **211**, 275 (1999).
- [2] **Ab initio study of the high-pressure phase transition from the cubic-diamond to the  $\beta$ -tin structure of Si**, K. Gaál-Nagy, M. Schmitt, P. Pavone, and D. Strauch, Comput. Mat. Science **22**, 49 (2001).
- [3] **Ab initio study of the enthalpy barriers of the high-pressure phase transition from the cubic-diamond to the  $\beta$ -tin structure of silicon and germanium**, K. Gaál-Nagy, A. Bauer, P. Pavone, and D. Strauch, Comput. Mat. Science **30**, 1 (2004).
- [4] **Ab initio study of the Imma phase in Silicon**, K. Gaál-Nagy and D. Strauch, Comput. Mat. Science **30**, 8 (2004).
- [5] **Ab initio study of the  $\beta$ -tin $\rightarrow$ Imma $\rightarrow$ sh phase transitions in silicon and germanium**, Katalin Gaál-Nagy, Pasquale Pavone, and Dieter Strauch, Phys. Rev. B **69**, 134112 (2004), see also arXiv:cond-mat/0308314.
- [6] **Druckinduzierte Phasenübergänge in Halbleitern mit *Ab-initio*-Methoden**, Katalin Gaál-Nagy, PhD thesis (in German language), Universität Regensburg, Germany (2004), URN: urn:nbn:de:bvb:355-opus-4008, URL: <http://www.opus-bayern.de/uni-regensburg/volltexte/2004/400/>.
- [7] **Phonons in the  $\beta$ -tin, Imma, and sh phases of Silicon from *ab initio* calculations**, Katalin Gaál-Nagy and Dieter Strauch, Phys. Rev. B **73**, 014117 (2006), see also arXiv:cond-mat/0502248.
- [8] **Transition pressures and enthalpy barriers for the cubic-diamond $\rightarrow$  $\beta$ -tin transition in Si and Ge under non-hydrostatic conditions**, Katalin Gaál-Nagy and Dieter Strauch, Phys. Rev. B **73**, 134101 (2006), see also arXiv:cond-mat/0508651.
- [9] **Theory and computation of electronic excitations in condensed matter systems: the ETSF project**, G. Onida, N. Manini, E. Mulazzi, A. Bordon, K. Gaál-Nagy, A. Incze, L. Caramella, M. Cazzaniga, E. Ponzio, A. Miglio, M. Gatti, CIMIANA, Milano (2006).
- [10] **Ab initio calculations of the optical properties of the Si(113) $3\times 2$  adatom-dimer-interstitial surface**, Katalin Gaál-Nagy and Giovanni Onida, Phys. Rev. B **75**, 155331 (2007), see also arXiv:cond-mat/0611124.

- [11] **Dielectric function of the Si(113) $3\times 2$ ADI surface from ab-initio methods**, Katalin Gaál-Nagy and Giovanni Onida, in *Epioptics, The Science and culture - Physics*, edited by A. Cricenti, (World Scientific, Singapore), **29**, 75 (2008), see also arXiv:cond-mat/0611121.
- [12] **First Principle Study of Silicon Nanocrystals: Structural and Electronic Properties, Absorption, Emission, and Doping**, Stefano Ossicini, O. Bisi, Elena Degoli, I Marri, Federico Iori, Eleonora Luppi, Rita Magri, Raffaele Poli, G. Cantele, D. Ninno, F. Trani, M. Marsili, O. Pulci, V. Olevano, M. Gatti, K. Gaal-Nagy, A. Incze, and G. Onida, *Jour. Nanoscience and Nanotechnology* **8**, 469 (2008).
- [13] **Ab-initio calculation of phonon dispersion curves: accelerating q point convergence**, Katalin Gaál-Nagy, *Phys. Rev. B* **77**, 024309 (2008), see also arXiv:0707.0384.
- [14] **Ab-initio calculation of the vibrational modes of SiH<sub>4</sub>, H<sub>2</sub>SiO, Si<sub>10</sub>H<sub>16</sub>, and Si<sub>10</sub>H<sub>14</sub>O**, Katalin Gaál-Nagy, Giulia Canevari, and Giovanni Onida, *Jour. Phys.: Cond. Mat.* **20**, 224013 (2008), see also arXiv:0708.3312.
- [15] **All-Optical determination of initial oxidation of Si(100) and its kinetics**, N. Witkowski, Yves Borensztein, O. Pluchery, Katalin Gaál-Nagy, A. Incze, Giovanni Onida, Frank Fuchs, Friedhelm Bechstedt, and Rodolfo Del Sole, *Eur. Phys. J. B* **66**, 427 (2008).
- [16] **Elementary structural building blocks encountered in silicon surface reconstructions**, Corsin Battaglia, Katalin Gaál-Nagy, Claude Monney, Clément Didiot, Eike Fabian Schwier, Michael Gunnar Garnier, Giovanni Onida, and Philipp Aebi, *J. Phys.: Condens. Matter* **21**, 013001 (2009), see also arXiv:0809.4961.
- [17] **Optical spectra and microscopic structure of the oxidized Si(100) surface: combined in-situ optical experiments and first principles calculations**, Katalin Gaál-Nagy, A. Incze, Giovanni Onida, Yves Borensztein, N. Witkowski, O. Pluchery, Frank Fuchs, Friedhelm Bechstedt, and Rodolfo Del Sole, *Phys. Rev. B* **79**, 045312 (2009).
- [18] **A new structural model for the Si(331)-(12x1) reconstruction** Corsin Battaglia, Claude Monney, Clément Didiot, Eike Fabian Schwier, Michael Gunnar Garnier, Philipp Aebi, Katalin Gaal-Nagy, and Giovanni Onida, *Phys. Rev. Lett.* **102**, 066102 (2009), see also arXiv:0807.3875.
- [19] **Ab initio absorption spectra of 3-tert-butylcyclohexene**, Katalin Gaál-Nagy, Olivia Pulci, and Giovanni Onida, *C. R. Physique* **10**, 491 (2009).

- [20] **Structure and stability of the Si(331)-(12×1) reconstruction**, Corsin Battaglia, Giovanni Onida, Katalin Gaál-Nagy, and Philipp Aebi, Phys. Rev. B **80**, 214102 (2009), see also arXiv\_0902.0774
- [21] **First-principles investigation of the vibrational properties of 3-tert-butylcyclohexene** Katalin Gaál-Nagy, Cent. Eur. J. Phys., accepted .
- [22] **Ab initio investigation of the groundstate, magnetic, electronic, and optical properties of polyynes and cumulene prototypes**, Carlo Motta, Marco Cazzaniga, Andrea Bordoni, and Katalin Gaál-Nagy, submitted, see also arXiv\_0904.2905.
- [23] **Implementation of optical matrix elements, including a real-space cutoff, to ABINIT**, Carlo Motta, Matteo Giantomassi, Marco Cazzaniga, Katalin Gaál-Nagy, and Xavier Gonze, submitted.
- [24] **Valence band structure of the Si(331)-(12×1) surface reconstruction**, Corsin Battaglia, Eike Fabian Schwier, Claude Monney, Clement Didiot, Nicola Mariotti, Katalin Gaál-Nagy, Giovanni Onida, Michael Gunnar Garnier, and Philipp Aebi, submitted.
- [25] **Thermodynamic properties of the  $\beta$ -tin, *Imma*, and sh phases in Silicon**, Katalin Gaál-Nagy, in preparation.
- [26] **Analysis of phonons of oxidized Si clusters from first principles methods**, Guido Fratesi, Giulia Canevari, Katalin Gaál-Nagy, and Giovanni Onida, in preparation.
- [27] **Analyze of the dielectric function of 3-tert-butylcyclohexene obtained from ab-initio calculations**, Katalin Gaál-Nagy *et al.*, in preparation.
- [28] **Analyze of soft phonons at the high-pressure  $\beta$ -tin, *Imma*, and sh phases of silicon from ab-initio calculations**, Katalin Gaál-Nagy, in preparation.
- [29] **Temperature dependence of the transition pressure for the  $\beta$ -tin  $\rightarrow$  *Imma*  $\rightarrow$  sh phase transitions in silicon**, Katalin Gaál-Nagy, in preparation.

Milan, May 16, 2010,

(Katalin Gaál-Nagy)