# Gerhard Kahl CURRICULUM VITAE

## Name

Gerhard Kahl

#### **Personal Information**

born on January 7<sup>th</sup> 1957 in Wien (Austria) married to Andrea Kahl; two children: Benedikt Maria and Christoph Maria

## **Present Position**

University Professor Director of the Institut für Theoretische Physik, TU Wien Director of the Viennese CECAM Node (Danube Center for Atomistic Modelling) Institut für Theoretische Physik and Center for Computational Materials Science (CMS) Technische Universität Wien (TU Wien) Wiedner Hauptstraße 8-10, A-1040 Wien, Austria

## Education & Studies

- Highschool (1967 1975)
- Technical Physics, Technische Universität Wien (1975 1979)
- PhD in Technical Sciences (Dr. techn.), Technische Universität Wien (1980 1983)
- Thesis: "On the Structure of Simple Liquids" (supervisor: J. Hafner)
- Formation for highschool teacher in mathematics and physics (1981 1985)
- Habilitation "Condensed Matter Theory", Technische Universität Wien, 1988

#### Academic Positions

- assistant (1980 1986): Institut für Theoretische Physik, TU Wien
- 'post-doc' (1987, 1988): Laboratoire de Physique Théorique des Liquides (J.-P. Hansen), Université Pierre et Marie Curie, Paris
- teacher-in-training (1988 1989): Lise Meitner Realgymnasium (Schottenbastei)
- assistant professor (since 1988): Institut für Theoretische Physik, TU Wien
- associate professor (1997): Institut für Theoretische Physik, TU Wien
- university professor (since 2011): Institut für Theoretische Physik, TU Wien

#### Academic Titles

Dipl. Ing. (1979), Dr. techn. (1984), Mag. rer.nat. (1986), Dozent (1988)

# Scholarships & Prices

- PhD "summa cum laude" ("sub auspiciis praesidentis rei publicae"; 1984)
- "Erich Schmid"-prize of the Österreichische Akademie der Wissenschaften (14.5.1986)
- $\circ~2\times$ "Ludwig-Wittgenstein"-scholarship of the Österreichische Forschungsgemeinschaft for young scientists (1984 1986)
- "Erwin Schrödinger"-scholarship of the Austrian Research Fund (FWF) (1986)
- Kardinal-Innitzer Förderungspreis (15.12.1994)

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#### **National Scientific Projects**

- FWF (J0156P) "Structure of liquid metals, liquid alloys and metal-salt solutions"
  - FWF (M0014-PHY; co-applicant) "A unified description of the liquid and gaseous phases of expanded liquid metals"
  - FWF (M0181-PHY; co-applicant) "Collective excitations in expanded liquid metals and insulating fluids"
  - FWF (M1170-N16; co-applicant) "Self-organization scenarios in inverse patchy colloid systems"
  - FWF (P7618-TEC) "Structure and thermodynamics of simple liquids and their mixtures"
  - FWF (P8912-PHY) "Elementary excitations in liquid metals"
  - FWF (P11194-PHY) "Density functional theory for confined fluids"
  - FWF (P13062-TPH) "Phase transitions in simple fluids"
  - FWF (P14371-TPH) "Structure, thermodynamics, and phase transitions in polydisperse liquid mixtures"
  - FWF (P15758-TPH) "Phase behaviour and criticality in simple fluids"
  - FWF (P17823-N08) "Phase transitions in soft matter systems"
  - FWF (P19890-N16) "Glass formation of colloids confined in porous materials"
  - FWF (P23910-N16) "Ordered structures in dipolar and ferrofluidic systems"
  - FWF (I2866-N36; co-applicant) "Self- assembly of DNA dendrimers in the bulk and at interfaces"
  - FWF (I2913-N27; submitted) "Competing length scales indriven confined fluids FWF (W004; co-applicant) Science College "Computational Materials Science"
  - FWF (F41; co-applicant) SFB "Vienna Computational Materials Laboratory"
- TU Wien (TU-Doktoratskolleg; speaker) "BioInterface"
- OENB (3204; co-applicant) "Theorie der Struktur der kondensierten Materie"
  OENB (4649) "Dynamic properties of liquid alkali metals"
  OENB (6241) "Structure en det envise of facilation generation and in and in a second secon
  - OENB (6241) "Structure and thermodynamics of fluids in porous media"
- Federal Ministry (co-applicant) "Atomic dynamics in liquid and glassy systems" Federal Ministry "TIPTOP – eine Informationsstruktur für die Physik" Federal Ministry "Structure, thermodynamics and phase behaviour in polydisperse liquid mixtures"
- o bilateral projects with France, United Kingdom, Slovenia, Czech Republic, Ukraine

# **Participation in European Projects**

- Member of the Management Committee of COST Action P13, "Forging the missing link: From Molecular Simulations to Nanoscale Experiments" – MOLSIMUL
- Member of the Management Committee of COST Action D43, "Colloid and Interface Chemistry for Nanotechnology"
- Member of the Management Committee of COST Action CM1101, "Colloidal Aspects of Nanoscience for Innovative Processes and Materials"
- Node-coordinator in the Marie Curie Initial Training Network (ITN) "Physics of Complex Colloids: Equilibrium and Driven" (COMPLOIDS)
- Director of the Viennese CECAM Node (Danube Center for Atomistic Modelling)

## **Conference Activities**

- Conference Secretary of the conference "Liquid and Amorphous Metals 8" (LAM8), Wien (Austria) August 1st - September 4th 1993
- Member of the Local Organizing Committee of the "Fifth Wigner Symposium", Wien (Austria) August 25th - 27th 1997
- Co-organizer of the CECAM-Workshop "Fluid phase behaviour and critical liquid state theory and simulations" (together with D. Pini and N.B. Wilding), Lyon (France), July 5th - 7th 2007
- Member of the Austrian Advisory Board of the "33rd Conference of the Middle European Cooperation in Statistical Physics – MECO33", Puchberg/Wels (Austria), April 14th -16th 2008
- Co-organizer of the CECAM-Workshop "New trends in simulating colloids: from models to applications" (together with G. Foffi and R. Vink), Lausanne (Switzerland), July 15th
   18th 2009
- Co-organizer of the CECAM-Workshop "Complex dynamics of fluids in disordered and crowded environments" (together with D. Coslovich and V. Krakoviack), Lausanne (Switzerland), June 26th - July 1st 2010
- Co-organizer of the Workshop "From Hamiltonians to phase diagrams" (together with G. Kresse), Wien (Austria), September 27th 29th 2010
- Co-organizer of the "8th Liquid Matter Conference LMC8", Wien (Austria), September 6th - 10th 2011
- Member of the Programm Committee of the 4th Conference "Statistical Physics: Modern Trends and Applications", Lviv (Ukraine), July 3rd - 6th 2012
- Co-organizer of the CECAM Workshop "Physics of colloidal particles with heterogeneously patterned surfaces (together with E. Bianchi, C.N. Likos, and F. Sciortino), Vienna (Austria), September 24th - 29th 2014
- Co-organizer of the workshop "Fluids in confinement: in- and out-of-equilibrium" (together with D. Coslovich), as part of the "14éme Journées de la Matière Condensée", Paris (France), August 24th - 29th 2014
- Co-organizer of the CECAM Workshop "Interactions and Transport of Charges Species in Bulk and at Interfaces (together with K. Kang, J. Dhont, and C.N. Likos), Vienna (Austria), July 4th - 7th 2016
- Co-organizer of the workshop "Design synthèse et assemblage de particules à patchs" (together with E. Bianchi, S. Ravaine, and E. Grelet), as part of the "15éme Journées de la Matière Condensée", Bordeaux (France), August 22th - 26th 2016
- Co-organizer of the CECAM Workshop "Structure formation in soft colloids (together with P. Ziherl), Vienna (Austria), September 19th - 22nd 2016
- Organizer of the CECAM Extended Software Development Workshop "Trajectory Sympling", Traunkirchen (Austria), November 16th 25th 2016

### Services to the Community

- Reviewer for the Austrian Academy of Sciences, Deutsche Forschungsgemeinschaft (DPG), Agence National de la Recherche (ANR), Slovenian Research Agency (ARRS), Fundação para a Ciência e a Tecnologia (FCT; Portugal), Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO; Niederlande), Department of Energy (DoE), Petrol Research Fund, Vetenskaprådet (Sweden), JSPS (Japan)
- Referee for Chemical Monthly, Chemical Physics Letters, Chemistry An Asian Journal, Colloid and Polymer Science, Colloids and Surfaces A, Condensed Matter Physics, European Journal of Physics E, Europhysics Letters, Fluid Phase Equilibria, International Journal of Molecular Sciences, Journal of Chemical Physics, Journal of Computational Chemistry, Journal of Molecular Simulation, Journal of Non-crystalline Solids, Journal of Physics A, Journal of Physics (Condensed Matter), JSTAT, Langmuir, Molecular Physics, Molecular Simulations, Nature Physics, Physica B, Physical Chemistry Chemical Physics, Physical Review B and E, Physical Review Letters, PNAS, Soft Matter
- Reviewer in PhD- and Habilitation-panels in Austria, Italy France, Spain, Germany, Sweden
- Member of the Liquids, soft matter and biological physics board of "The Journal of Physics (Condensed Matter)"

Guest Editor in "Molecular Physics" and Journal of Physics (Condensed Matter)

# Member in Scientific Organizsations

- Member of the Austrian Physical Society (ÖPG)
- Member of the "Center for Computational Materials Science" (CMS)
- Founding member of the Science College "Computational Material Science"
- Austrian Representative at the "Scientia Europæa Conference" (Fondation Rhône-Poulenc de l'Institut de France)
- President of the Austrian Chemical Physical Society (CPG) 2003/2004

# **Research Interests**

During the past years our scientific activities have focused on the investigations of the static, dynamic, and self-assembly properties of soft matter systems, with particular emphasis on colloidal dispersions. Our research is based on a broad variety of statistical mechanics based techniques or concepts, ranging from integral-equation approaches, over classical density functional theory, mode coupling theory, computer simulations, to optimization strategies based on ideas of genetic algorithms.

Typically, our investigations start from a monomer resolved model for colloidal particles (such as dendrimers, polymers, etc.) for which we derive via suitable coarse-graining approaches effective interactions, that also take the surrounding solvent into account. Based on these interparticle potentials we evaluate structural and thermodynamic properties of the system, with particular emphasis on the phase diagram. Special focus is put on characteristic self-assembly scenarios, such as clustering phenomena or the identification of ordered equilibrium structures. Furthermore we study the dynamic properties of colloidal systems, investigating possible dynamical arrest scenarios. Recent efforts have been dedicated to soft systems under confinement, whereby the latter can be realized either via limiting walls or via disordered, quenched particle configurations as they are encountered in porous systems.