

MM 8: Topical Session: Quasicrystals & Complex Metallic Alloys II

Time: Monday 11:45–13:00

Location: H25

MM 8.1 Mon 11:45 H25

Electronic Wave Functions of Quasiperiodic Systems in Momentum Space — ●STEFANIE THIEM, SEBASTIAN ROLOF, and MICHAEL SCHREIBER — Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany

In quasicrystalline tilings often multifractal electronic wave functions can be found, which are neither extended over the whole system nor exponentially localized. In order to obtain a better insight into their localization properties, we study the wave functions of quasiperiodic tilings in momentum space. The models are based on one-dimensional quasiperiodic chains, in which the atoms are coupled by weak and strong bonds aligned according to the Fibonacci sequences. The associated hypercubic tilings and labyrinth tilings in d dimensions are then constructed from the direct product of d such chains.

The results show that each wave function is described by a hierarchy of wave vectors and is always dominated by a single wave vector which is directly related to the energy eigenvalue of the wave function. Combining the information of all wave functions of the system, we observe a hierarchy of branches with different intensities. Each branch is a copy of the main branch containing the dominant wave vectors for each wave function. Using perturbation theory and a renormalization group approach we determine the shape of the branches for the limit cases of weak and strong coupling.

MM 8.2 Mon 12:00 H25

Confirmation of the Random Tiling Hypothesis for a Decagonal Quasicrystal — ●ALEXANDER KISELEV¹, MICHAEL ENGEL², and HANS-RAINER TREBIN¹ — ¹Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany — ²Department of Chemical Engineering, University of Michigan, USA

The random tiling hypothesis of Henley and Elser states, that the configurational entropy due to the phason flips stabilizes a quasicrystal at elevated temperatures and leads to a periodic crystal at low temperatures. Here, we study the role of entropy for a monatomic two-dimensional decagonal model quasicrystal, whose atoms interact by a double-well Lennard-Jones-Gauss pair potential. We calculate the free energy of the system, which can be split up into a phonon part and a configurational part. The phonon part of the free energy is calculated with molecular dynamics using the Frenkel-Ladd method. For the configurational part a new Ising-type model of uncorrelated flips is employed in Monte Carlo simulations. We observe that the free energy takes a square-gradient form of the phason displacement as predicted by the random tiling hypothesis and determine phason elastic constants over a large range of temperatures. The free energy calculations confirm a phase transition from an entropically stabilized decagonal random tiling phase to an energetically stabilized periodic crystal. Thus, for the first time, a virtual quasicrystal confirms all predictions of the random tiling hypothesis in a fully atomistic model [1].

[1] A. Kiselev, M. Engel and H.-R. Trebin, arXiv:1210.4227 (2012)

Topical Talk

MM 8.3 Mon 12:15 H25

Self-assembly and packing of polyhedra into complex crystal structures — ●MICHAEL ENGEL¹, PABLO F. DAMASCENO¹, AMIR HAJI-AKBARI², and SHARON C. GLOTZER¹ — ¹Chemical Engineering, University of Michigan, USA — ²Chemical and Biological Engineering, Princeton University, USA

Isolating the role of building block shape for self-assembly and packing provides insight into the ordering of molecules and the crystallization of colloids, nanoparticles, proteins, and viruses. We investigated a large group of polyhedra whose phase behavior arises solely from their anisotropic shape by exploiting entropic driving forces. Our results demonstrate a remarkably high propensity for thermodynamic self-assembly and structural diversity [1]. In particular, I will discuss the formation and geometric stabilization of a dodecagonal quasicrystal with tetrahedra [2] as well as the appearance of topologically close-packed phases. All of the crystal structures we observe have analogues in the elements and can be understood by relating shape to atomic interactions. It turns out that the structural complexity is particularly high, when entropy and geometric constraints compete with locally dense configurations.

[1] P.F. Damasceno et al. Science 337, 453 (2012)

[2] A. Haji-Akbari et al. Nature 462, 773 (2009)

MM 8.4 Mon 12:45 H25

Symmetry and Chemistry of Complex Intermetallics — ●JULIA DSHEMUCHADSE and WALTER STEURER — Laboratory of Crystallography, Department of Materials, ETH Zurich, Switzerland

Complex intermetallic structures can be found in many different systems and exhibit giant unit cells. They feature a number of peculiar properties, but until recently, no unifying approach has been applied to describe their structures. To achieve a deeper understanding of their building principles, we are examining the structures of complex intermetallics on three different levels. For a generalized definition, we are statistically comparing the distribution of complex intermetallics over the entirety of intermetallic structures. Secondly, we have picked out highly symmetric lattices (*e.g.*, [1]), which feature a large number of complex structures, and analyze the distribution of different structure types within these groups, as well as their interrelations. The third step focuses on specific intermetallic systems featuring multiple complex compounds and describes their special geometries in a comparative way to reveal similarities and distinctions.

By trying to better understand complex intermetallic structures, we hope to be able to gain more profound knowledge on the formation of metallic matter in general.

[1] J. Dshemuchadse, D. Y. Jung, W. Steurer, Acta Cryst. B67, 269-292 (2011).