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From missions to Mars to twisted bilayer graphene; moiré patterns, higher order coincidences, number theory and using Python to solve these problems.

Date: 2023/04/25 (Tue)
Venue: S4-625
Time: 14:00-16:00

Abstract:
When rotational epitaxy phenomenon were first studied, the preferences for layers atoms of certain materials to arrange themselves at specific angles were explained in terms of energy minimization and relaxation. For arrangements without higher order coincidences, energetically preferred angles were possible only if atomic positions could relax slightly, with some interatomic distances larger than others.

Work in this area experienced a powerful resurgence following two major events in surface science – the breakthrough discovery and development of hexagonal/honecomb xene materials like graphene on hexagonal crystal surfaces, and the discovery that homo- and heterostructured 2D layered structures rotated at very small angles of order 1 degree resulted in unexpected emergent properties such as superconductivity.

While the details of mechanisms are still hotly debated, it is agreed that it is the production of moiré patterns due to small angle rotations or small mismatches in lattice constants within the multilayer structures producing a long-range modulated potential. The first and most famous of these situations is of course twisted bilayer graphene, but like everything in 2D materials, “What happens in graphene, stays in graphene[1]” absolutely does not apply!

In my talk I will start with the concept of a moiré pattern in 1D and expand to 2D square and hexagonal patters so we can get a feel for the moiré lattice. Then I’ll explain the basic mathematics behind it, from the reason that launches of space missions to the planet Mars come in clusters every 2.14 years, to the reasons that theorists think the “magic angles” of twisted bilayer graphene start at 1.1° and decrease, why 30° twisted bilayer graphene is considered as a quasicrystal, and why bilayer graphene higher order coincidences (HOCs) configurations nearby magic angles are so important for theorists.

Finally, I’ll explain our current work on HOCs. Touching on concepts in number theory and working in the complex plane we’ll see the “Universal Hex-on-Hex HOC map” and look at several recent experimental published examples of these HOCs observed in Low Energy Electron Diffraction (LEED) images.

[1] https://en.wikipedia.org/wiki/What_Happens_Here,_Stays_Here