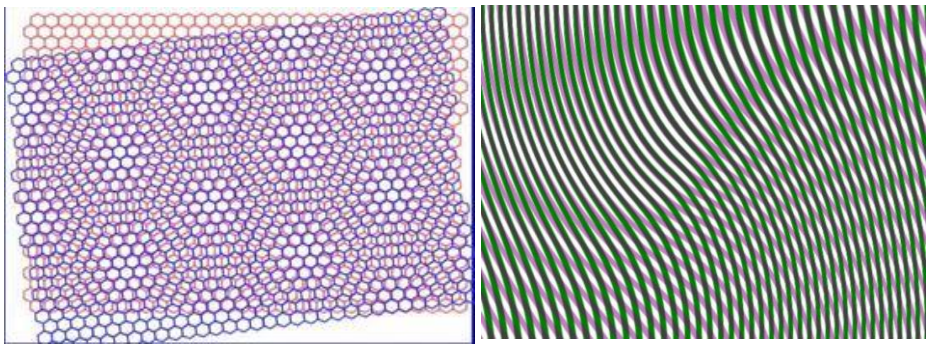
Moire patterns, shown on the picture, are large scale interference effects that appear when two periodic lattices, that are either not exactly commensurate or tilted with respect to each other, are overlaid. We frequently meet them in everyday life, they are aesthetically intriguing, attracting the long-standing attention of artists, and also causing havoc for inexperienced photographers. Remarkably, very recently scientists were able to create the same phenomenon on the smallest possible scale- the scale of atoms. For around two decades now we have witnessed an explosion of interest in 2D materials – flakes of materials that are only one atom thick – and it has not escaped the attention of aesthetically inclined researchers, that by overlaying two flakes there is a chance to create the smallest possible Moire pattern. The result has exceeded all expectations. By creating the Moire pattern, we have discovered a whole new world of phenomena, where the two flakes that separately are just seemingly boring metals, when brought together at a small tilt angle become superconductors or can host orderings such as magnetism or ferroelectricity. This is all very exciting, because Moire structures turn out to be not only aesthetically appealing, but also pave an unexpected way for new functionalities. One can imagine creating the smallest possible, two atoms thick, magnets that can be incorporated as smallest switches, for instance to activate medicines in-vivo.



However, there is one problem. Small angle Moiré structures, while extremely tiny from our macroscopic perspective, are in fact quite huge from the point of view of single atoms. One needs to account for thousands of atoms to see the Moiré pattern in its full glory and also to harvest fully its emergent properties. We need a theoretical method to describe it, but atomistic, quantum mechanics method, even averaged ones, are computationally too costly. Actually, this problem with Moiré patterns belongs to a much wider class of mesoscopic problems, where we are able to create structures with dimensions of tenths of nanometers, but we cannot really describe their stability -- the way atoms can re-arrange, so that one atomic structure can turn into another by a local tilt angle relaxation. One can entirely forget about details and treat atoms simply as classical balls, but with this simplification all chemical information about the atoms are lost and carbon becomes the same as silicon or tin. While experiments tell us that there is an exciting variability to explore there, e.g. that only some chemical compositions lead to Moiré's magnetism, while other do not.

The question is then: can we provide a method for describing such mesoscopic structures that one one hand can capture atomistically huge systems while on the other will have a sufficient insight into the properties of each atomic site. And moreover it will be simple enough to be satisfying for engineers creating new devices. In our research, computational scientists and solid state physicists will team up together to provide an affirmative answer to this question. Our aim is to derive an optimal method to tackle this problem and check if we are able to provide distinct predictions for 2D flakes made out of different elements. Ultimately, we hope to build a link with experiments and in this way find a more profound understanding why the Moiré patterns are so intriguing for us.