

**Title**

Elemental 2D materials beyond graphene: Insights from computational theory

**Abstract**

The presentation will address recent developments related to elemental 2D materials beyond graphene, with a focus on silicene, germanene, and arsenene. Several examples will be discussed in order to illustrate how computational theory based on first-principles calculations can contribute to understanding basic physical and chemical phenomena in 2D condensed matter. Silicene is of particular interest due to its compatibility with established Si technology. Regrettably, strong interaction with common substrates eliminates the Dirac states. Alternative substrates will be analyzed and the effects on silicene evaluated with respect to technological requirements. Germanene attracts more and more attention, because effects of spin-orbit coupling are accessible in contrast to lighter 2D materials. While the same is true for arsenene, the material's strongly buckled structure is not compatible with Dirac physics. Recovering the  $sp^2$  bonding, on the other hand, makes it possible to realize unusual properties.

**Biography**

Dr. Schwingenschlögl is a Professor of Materials Science & Engineering at King Abdullah University of Science and Technology (KAUST). His research interests in condensed matter physics and first-principles materials modeling focus on two-dimensional materials, interface and defect physics, correlated materials, thermoelectric materials, metal-ion batteries, nanoparticles, and quantum transport. Dr. Schwingenschlögl joined KAUST as founding faculty member in 2008, having previously worked at the International Center of Condensed Matter Physics in Brasilia, Brazil, and the Universität Augsburg in Germany.