ELASTIC PROPERTIES OF HYDROGENATED GRAPHENE: A BLENDED CONTINUUM/ATOMISTIC INVESTIGATION

L. Colombo[a]

[a]Department of Physics, University of Cagliari (Italy)

There exist three crystalline conformers of hydrogenated graphene, referred to as chair-, boat-, or washboard-graphane, all characterized by a C:H ratio equal to 1. These two-dimensional periodic materials are still mapped onto the graphene scaffold but they are characterized by a different orbital hybridization. Another possible form of hydrogenated graphene is fully disordered, corresponding to a C:H ratio smaller than 1. By blending together continuum elasticity and first-principles calculations [1], we determine the linear and nonlinear elastic moduli of all graphane conformers and provide evidence that they respond to any arbitrarily oriented extension with a much smaller lateral contraction than graphene. Interestingly enough, we find that boat-graphane shows a small and negative Poisson ratio (or, equivalently, an axially auxetic elastic behavior), while chair-graphane admits both softening and hardening hyperelasticity, depending on the direction of applied load. Finally, preliminary results on the elastic moduli of disordered hydrogenated graphene are presented and discussed in the linear response regime [2].

References

[1] E. Cadelano, P.L. Palla, S. Giordano, L. Colombo, Phys. Rev. B, 82 (2010) 235414.
[2] E. Cadelano and L. Colombo, in prepraration (2011)