

# **Complex absorbing potential in the framework of GKS-spRPA theory : Application to negative ion resonances**

*Abhisek Ghosal*

Many anions found in nature are stable i.e., the neutral molecule is able to bind extra electrons despite the repulsion by the other electrons. From a theoretical point of view, negative ion resonances, which bind one or several extra electrons only temporarily, are much more interesting. They are observed in radioactive decays, dissociative electron attachment, stark ionisation, even in bio-molecules like nucleotides, etc. Since the systems are temporarily resonance with the continuum, this can be rationalised by the difficulty of treating the many-body problem and the scattering continuum at the same time. The density functional theory (DFT) based GKS-spRPA method shows that nonlocal correlation effect is important in understanding electron molecule interaction for bound anions. However for unbound anions, such as the negative ion resonances, the impact of nonlocal correlation is unknown due to lack of theoretical framework. Here we develop a practical framework to study the negative ion resonances by introducing a local complex absorbing potential (CAP) in the GKS-spRPA energy functional. The new method, CAP-GKS-spRPA is able to treat both continuum and non-local correlation effects simultaneously. We observed that it shows remarkable improvement in the description of negative ion resonances compared to its exact exchange based method. Additionally, our method gives the resonance energy parameters within 0.2 eV as compared to the state-of-the-art CAP-EOM-EA-CCSD method. This work provides a practical solution to long-standing issue of characterising negative ion resonances within the GKS-DFT framework in a non-empirical fashion.