INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Thesis Title: **Application of Modified Smooth Exterior Scaling Method to Study Auger and Shape Resonances in Different Atomic and Molecular Systems.**

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SHORT ABSTRACT

This thesis focuses on the application of modified smooth exterior scaling (MSES) as an efficient method to impose outgoing boundary conditions in e-atom and e-molecule scattering resonances. This is the first time that the MSES method has been applied to calculate energies and widths of Auger and shape resonances in three-dimensional many-body electron systems. MSES converts the divergent resonance wave functions into square integrable ones thereby making the study of temporary bound states (resonance states) amenable to bound state electronic structure methods. The main objective of this thesis is to formulate the MSES method in bivariational SCF and electron propagator methods.

The shape resonances of isoelectronic systems $^2\Pi_g$ N_2^- and $^2\Pi$ CO^- have been studied to test the efficacy of the MSES method in the case of e-molecule scattering shape resonances. Then, the Auger and shape resonances of Be atom are investigated to test the method in the case of e-atom scattering Auger and shape resonances. The dilated electron propagator (dilated by MSES) is used up to second order in the case of molecular systems and up to third order in the case of atomic systems. The resonance energies and widths obtained from our calculations are in good agreement with experimental results and other theoretical estimates available in the literature. Further, we have also characterized the effects of diffused functions in characterizing the molecular shape resonances. From this investigation, it is observed that the additional p-type functions have an important role in characterizing the molecular shape resonances. However, the s- and d-type functions have negligible impact. Therefore, the basis set convergence can be obtained by adding additional diffused p-type functions to standard basis sets. Moreover, it is also observed that additional diffused functions, especially the p-type function, must be added to the standard basis sets while applying the MSES method in characterizing shape resonances.