

# Electronic structure investigation of Solvated Electron Precursors with *ab initio* calculations

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Solvated Electron Precursors (SEP) represent a unique class of molecules with delocalized electrons at the periphery of metal-ammonia complex. These systems stand out as pseudo-hydrogen atoms with pseudo-nuclei formed by the metal-center, ammonia ligands, and s-type orbital electrons shared across the entire molecule [J, Phys. Chem. Lett. 9(1): 84-88 (2018)]. The pseudo-atomic nature of SEPs and the diffuse character of peripheral electron make them promising for quantum computing hardware applications.

In this work we present geometric and electronic structure information for the  $(\text{NH}_3)_{3-5}\text{MgCH}_3$  complexes, and their dimers linked via hydrocarbon chains with different lengths (1-10 carbon atoms). Optimized geometries and frequencies are reported for triplet, open-, and closed shell singlet electronic configurations using *density functional theory* (DFT/CAM-B3LYP) combined with an augmented cc-pVTZ basis set for hydrogen atoms and cc-pVTZ basis sets for all other atoms. All molecular structures resulting from these calculations are stable and have no imaginary frequencies. Using these optimal geometries of each monomer and dimer, a series of electronically excited states are examined employing *multi-reference methods* (CASSCF and CASPT2) with the same basis sets.

Our results, aside from general molecular and electronic structure properties of Mg-SEPs, shed light on the prospect of their application in quantum computing hardware.