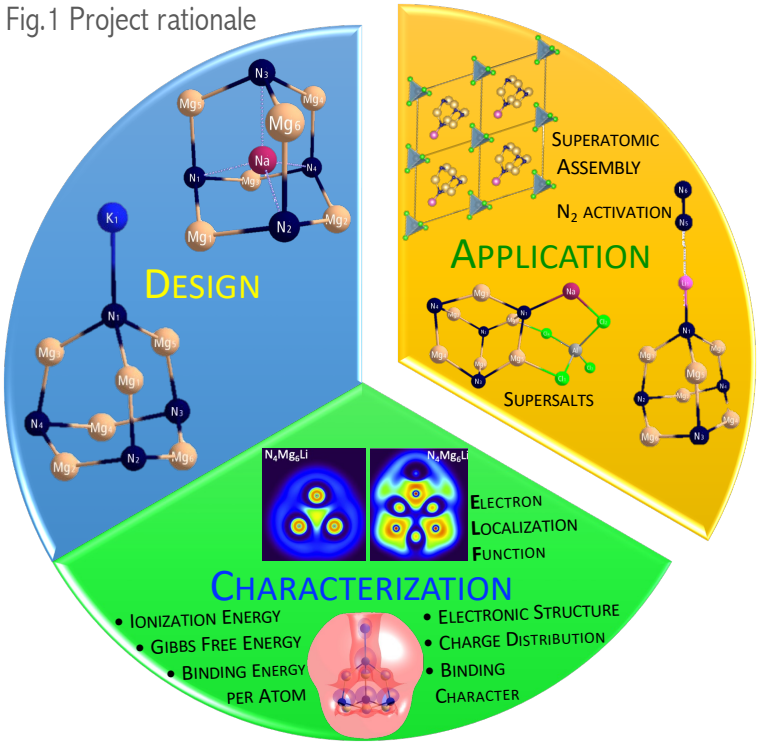
Superatoms are clusters of atoms that act like a single atom.[1-3] They have unique properties, including diverse functionalization, redox activity, and magnetic ordering. Materials made up of superatoms, so-called cluster-assembled solids, hold the promise of high tunability, atomic precision, and robust architectures. Superalkalis are a class of superatoms that have extremely low ionization energy and might serve as reducing agents. [4-6] In this project, we will **design new superalkalis and examine their chemical applications.**

Earth-abundant nitrogen (N_2) is a cheap, nontoxic, and abundant nitrogenous feedstock. The Haber-Bosch process is the predominant source of the world's ammonia (NH_3) production (of 175 million metric tons) and represents more than 90% of the annual production. Despite significant efforts in optimizing the process, it still consumes 1 to 2% of the worldwide annual energy for the high-working temperatures (at 573-873 K) and pressures (at 100-360 atm), currently producing more than 1.6% of global CO_2 emissions. So, developing efficient catalysts that convert N_2 into ammonia is vital to reduce the growing energy crisis and global warming. Chemical activation of N_2 by catalysts is a crucial step towards producing NH_3 efficiently and economically. The high stability of N_2 makes the conversion difficult. This is a challenging transformation as N_2 has a N≡N triple bond and the activation energy is high (941 kJ/mol). The goal of this project is to design and explore **superalkalis for N_2 activation and conversion into ammonia**.

Using a computational (*in silico*) approach and quantum mechanical techniques, we will realize the following research objectives (Fig.1):

- Design new superalkalis and investigate their physicochemical characterization.
- Design cluster assembled materials and examine their optoelectronic properties.
- Determine the best candidate for N_2 reduction reaction and examine the subsequent reactions of activated N_2 that lead to its transformation into ammonia (NH_3).

Fig.1 Project rationale



We believe that the electronic properties of superalkalis can predict the efficiency of superalkali/N_2 complex formation. We will investigate the influence of electronic structure, ionization energy, and geometric structure on the stability and selectivity of superalkali/N_2 complexes. The results of this project will enhance our understanding of N_2 conversion into ammonia. Subsequently, this can be used to develop a pathway for sustainable nitrogen molecule utilization and fertilizer shortage reduction.

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