

Chemical Design for Optical Cycling Centers

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Optical Cycling Centers (OCC) are functional groups that can be used for laser cooling, in the field of quantum information science. OCCs are characterized by having localized and isolated electronic states within a polyatomic molecule, which can be used to repeatedly excite and de-excite the molecule in a controlled photon-mediated regime. [1–3] Recent advances have shown that laser cooling can be extended to polyatomic molecules with polarized metal-oxygen bonds with metal-centered electron acting as a platform for OCC. Increasing system’s complexity provides new avenues for control of OCC’s electronic and vibronic properties, and it has been shown that increasing system’s size to more than three atoms potentially does not hinder its ability to be laser cooled. [4] Here we present several candidates for laser cooling applications based on highly-ionic M(I)-O bond and shielded $f \rightarrow f$ transition motifs. [5, 6] We demonstrate how conventional chemical design rules can be applied to these systems, using symmetry, bond character, and system size to manipulate the electronic properties of the OCC, and systematically improve their vibronic properties. We also developed methods suitable for screening these systems, potentially allowing for tuning the system’s properties for a variety of applications. Secondly, we present a principally different quantum functional moiety – an Yb3+ cation shielded by a rigid ligand in solution. Through the ligand and solvent engineering, these complexes can achieve the record-narrow electronic transitions in solution phase at room temperature, paving the way to quantum sensing that rivals atomic vapor cells.

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