

---

# Probing local structures and dynamics in emerging materials for optoelectronics and photovoltaics

G N Manjunatha Reddy\*<sup>1</sup>

<sup>1</sup>University of Lille – Univ. Lille, CNRS, Centrale Lille, ENSCL, Univ. Artois, UMR 8181 - UCCS - Unité de Catalyse et Chimie du Solide, F-59000 Lille, France – Lille, F-59000, France

## Résumé

The past five years have seen significant fundamental and technological advancements in the solution-processable semiconductor materials for solar energy conversion. Specifically, organic semiconductors (OSCs) and hybrid halide perovskites (HPs) are promising light harvesting materials among the emerging photovoltaic technologies today. For example, single-junction solar cells based on OSCs and HPs have achieved solar-to-electrical energy conversion efficiencies of over 18% and 25%, respectively, compared to the theoretical Shockley-Queisser limit of 33%. While this trend is expected to continue, the energy harvesting capability of these materials is not withstanding to provide with sustainable large area photovoltaic platform in the long run, due to the poor environmental stability and degradation issues. What becomes clear as the field develops is that the compositional engineering of photoactive layers and contact electrodes, and their interfaces, is increasingly important to develop stable and efficient solar cells. In addition, acquiring deep new understandings of structure-stability-property relationships is expected to help in the rational design of solution-processable semiconductor materials for optoelectronics. Here, we present the general application of solid-state NMR (ssNMR) spectroscopy to characterize organic-organic interfaces in OSCs and organic-inorganic interfaces in HPs.[1-4] Results on multi-nuclear (<sup>1</sup>H, <sup>13</sup>C, <sup>11</sup>B, <sup>14</sup>N/<sup>15</sup>N, <sup>19</sup>F, <sup>119</sup>Sn, <sup>133</sup>Cs, and <sup>207</sup>Pb) ssNMR characterization of organic photovoltaic blends and hybrid perovskites will be presented.

## References:

M. Seifrid et al., Nature Reviews Materials, 2020, 5, 910-930 A. Karki et al., Energy & Environmental Science, 2020, 13, 3679-3692 A. Krishna et al., Advanced Functional Materials. 2020, 30, 1909737. C. Dahlman et al., Chemistry of Materials, 2021, 33, 642-656

---

\*Intervenant