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Making Flying Greener: A machine intelligence perspective

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Despite all advances in sustainable alternatives for the transportation sector (hydrogen, battery), diesel and kerosene will continue to be used for mobility in the foreseeable future, mainly for long-haul applications such as shipping, aviation, and trucking. This is an undeniable truth, and rather than attempting to fight against it, AI can help make it greener. The aviation industry is particularly challenging to decarbonise due to its use of high-energy-density fossil jet fuels. Designing sustainable aviation fuels with performance characteristics and operability limits to act as a drop-in is essential in this context. This work presents an advanced *De Novo fuel discovery AI framework* to develop sustainable aviation fuels that meet the high energy density requirements of the aviation sector, as shown in Fig. 1. The fuel design approach is built upon a deep kernel learning model to develop quantitative structure-property relationship models to predict the physicochemical properties of pure compounds and fuel blends with confidence bounds required for decision-making tasks. The deep kernel learning model is then integrated into an inverse design framework to explore novel sustainable aviation fuel compositions according to performance targets. The AI framework can potentially lead to sustainable aviation fuels fully compatible with the existing aircraft infrastructure.

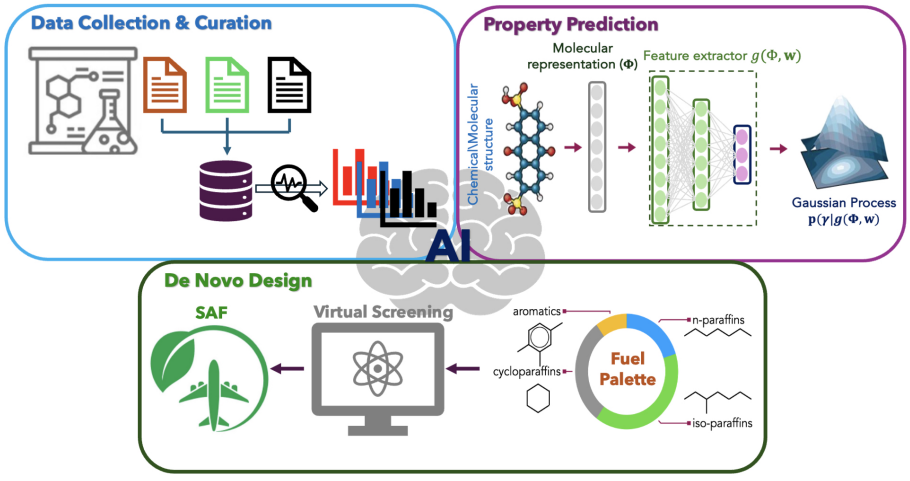

Figure 1: **De Novo fuel composition discovery**. An AI-assisted framework for exploring sustainable aviation fue