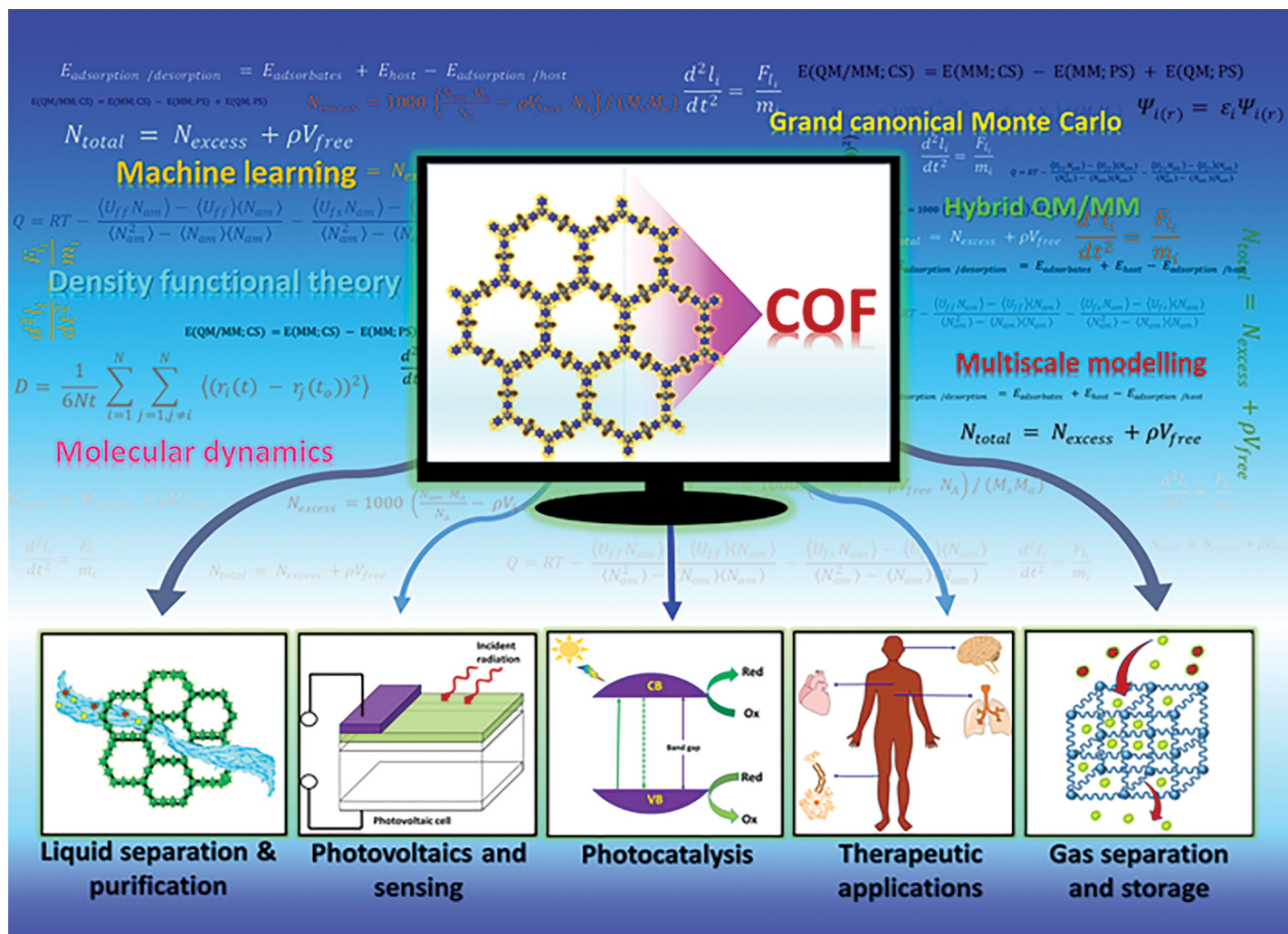


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Exploring covalent organic frameworks through the lens of computational chemistry

The review explores the critical role of computational chemistry during the design, modelling, and applications of COFs, unveiling their exciting potential and providing a profound understanding of the existing experimental and hypothetical COFs at the atomic scale. Emphasizing the key challenges and future perspectives, this review may serve as a stepping stone for future advancements that ultimately guide the design and development of COF-based tailored materials for their ubiquitous applications in research and industrial domains, thereby mitigating current challenges.

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