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Ab-initio Calculations on the Mechanism of Action of Platinum and Ruthenium Complexes in Phototherapy

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Abstract : The medical techniques based on the use of light for activating the drug are occupying a prominent place in the cancer treatment due to their selectivity that contributes to reduce undesirable side effects of conventional chemotherapy. Among these therapeutic treatments, photodynamic therapy (PDT) and photoactivated chemotherapy (PACT) are emerging as complementary approaches for selective destruction of neoplastic tissue through direct cellular damage. Both techniques rely on the employment of a molecule, photosensitizer (PS), able to absorb within the so-called therapeutic window. Thus, the exposure to light of otherwise inert molecules promotes the population of excited states of the drug, that in PDT are able to produce the cytotoxic species, such as 1O2 and other ROS, in PACT can be responsible of the active species release or formation. Following the success of cisplatin in conventional treatments, many other transition metal complexes were explored as anticancer agents for applications in different medical approaches, including PDT and PACT, in order to improve their chemical, biological and photophysical properties. In this field, several crucial characteristics of candidate PSs can be accurately predicted from first principle calculations, especially in the framework of density functional theory and its time-dependent formulation, contributing to the understanding of the entire photochemical pathways involved which can ultimately help in improving the efficiency of a drug. A brief overview of the outcomes on some platinum and ruthenium-based PSs proposed for the application in the two phototherapies will be provided.

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