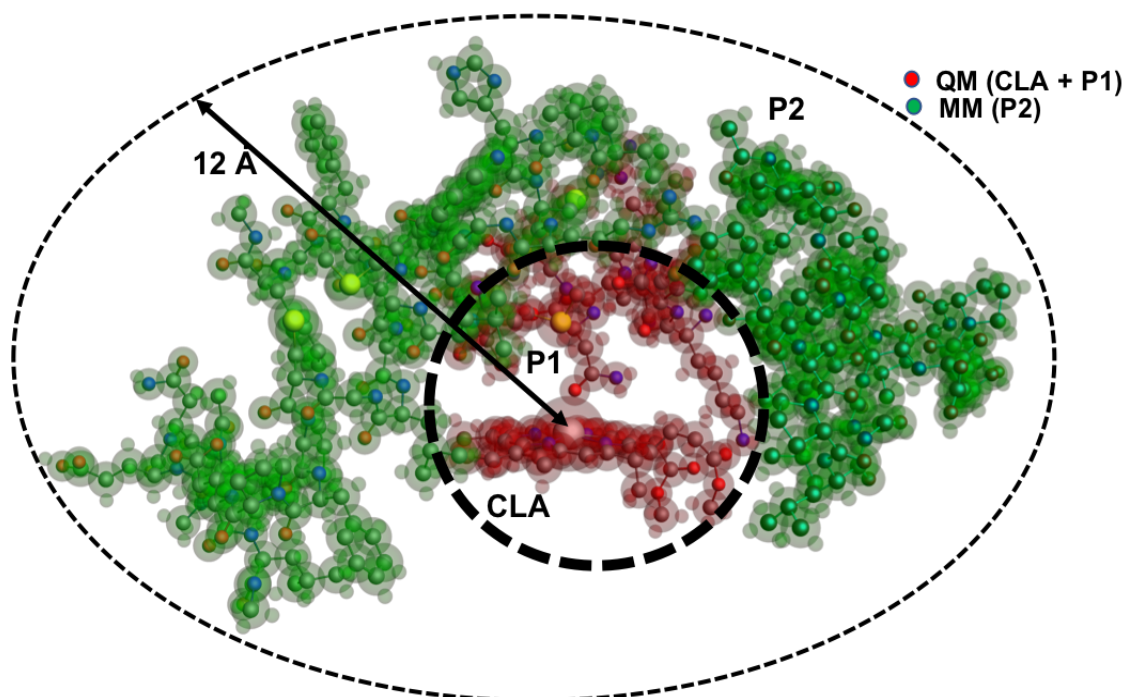


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Light Harvesting Complex II (LHCII) is one of the major pigment complexes in higher plants largely responsible for light absorption and energy transfer. Studies have shown that LHCII can switch its functionality between a photo-active and a photo-quenched state, manifested by a change in the conformation and excitonic interaction between the chlorophyll and carotenoids. In order to study the effect of the protein environment on the absorption energy of chlorophyll, we focused on a putative quenching site as proposed previously and established an optimum full protein model which could be treated accurately and at the same time describing the electrostatics involved in protein dynamics. Starting with the crystal structure we selected an environment of 12 Å around the Mg center of a chlorophyll a (denoted hereby as CLA612) at the quenching site and modelled it using different QM and QM/MM techniques. We divided the environment depending on the proximity of the residues to the chlorophyll. We treated the nearby residues in an accurate QM way and the far away residues in a more approximate way using point charges and polarizabilities under the Discrete Reaction Field (DRF) model. On comparing our results, we concluded that the far away residues do not have any direct and significant effect upon the absorption energy as long as we do not distort the crystal structure and produce artefacts in the structure.



## References

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