Simulations of Ion Solvation and Transfer by Adaptive-Partitioning QM/MM Dynamics

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Ion solvation and transport is important to many physical, organic, and biochemical processes. However, the frequent exchange of solvent molecules between the ion's solvation shell and the bulk solvent presents a challenge for combined quantum-mechanics/molecular mechanics (QM/MM) simulations. Adaptive-partitioning QM/MM allows on-the-fly reclassification of atoms as QM or MM both continuously and smoothly.[1] This permits the use of a small, mobile QM subsystem, with contents that are updated as needed when the trajectory is propagated. In this talk, we report our latest progress in the development of adaptive-partitioning QM/MM strategies (Fig. 1) for simulations of proton transfer through a prototypical chloride/proton antiporter.[2]

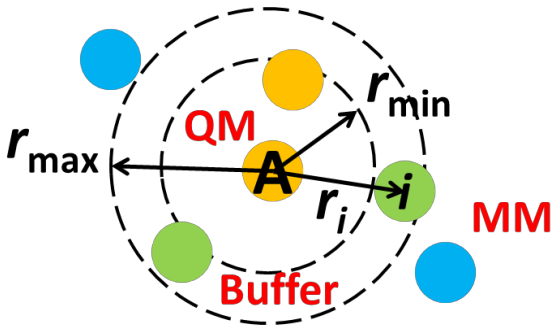

Fig 1. Schematic of adaptive-partitioning QM/MM. The QM zone is centred at a selected molecule or ion A. The distance r_i between a buffer group i and the QM-zone centre satisfies $r_{\max} \geq r_i \geq r_{\min}$. The QM, buffer, and MM groups are coloured in orange, green, and blue, respectively.

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References

[1] Duster, A. W.; Wang, C.-H.; Garza, C.; Miller, D.; Lin, H. "Adaptive QM/MM: Where are we, what have we learned, and where will we go from here?" *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2017**, *7*, e1310.

[2] Duster, A. W.; Garza, C. M.; Aydintug, B. O; Negussie, M. B.; Lin, H. "Adaptive partitioning QM/MM for molecular dynamics simulations: 6. Proton transport through a biological channel," *Journal of Chemical Theory and Computation*, **2019**, *15*, 892-905.