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Electronic coarse graining enhances the predictive power of molecular simulation allowing challenges in water physics to be addressed

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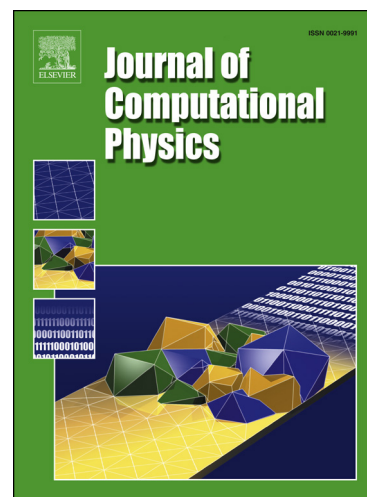
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Graphical abstract

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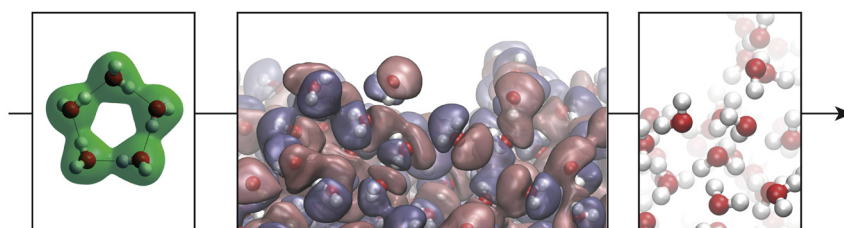
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Electronically coarse-grained methods bridge
ab initio calculations and all-atom molecular dynamics



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