

Table 1: Different Models to Calculate Electrostatic Potential Energy of QM/MM under Periodic Boundary Conditions

Embedding _≤ Embedding _{>}	EEd EEd	EEd EEd'	EEd EEd''	EEd EEq	EEd EEq'	EEd ME	EEq EEq	EEq EEq'	EEq ME	ME ME	EEd	EEq	ME
$\langle \rho_{QM} \hat{J}_{\leq} \rho_{QM} \rangle$	•	•	•	•	•	•	•	•	•	•	•	•	•
$\langle \rho_{QM} \hat{J}_{\leq} q_{MM} \rangle$	•	•	•	○	○	○					•		
$\langle Q_{QM} \hat{J}_{\leq} q_{MM} \rangle$				○	○		•	•	○			•	
$\langle Q_{QM}^{ref} \hat{J}_{\leq} q_{MM} \rangle$						○			○	•			•
$\langle \rho_{QM} \hat{J}_{>} \rho_{QM} \rangle$	•												
$\langle \rho_{QM} \hat{J}_{>} Q_{QM} \rangle$		•											
$\langle \rho_{QM} \hat{J}_{>} Q_{QM}^{ref} \rangle$			•										
$\langle Q_{QM} \hat{J}_{>} Q_{QM} \rangle$				•			•						
$\langle Q_{QM} \hat{J}_{>} Q_{QM}^{ref} \rangle$					•			•					
$\langle Q_{QM}^{ref} \hat{J}_{>} Q_{QM}^{ref} \rangle$						•			•	•			
$\langle \rho_{QM} \hat{J}_{>} q_{MM} \rangle$	•	•	•										
$\langle Q_{QM} \hat{J}_{>} q_{MM} \rangle$				•	•		•	•					
$\langle Q_{QM}^{ref} \hat{J}_{>} q_{MM} \rangle$						•			•	•			
Comments			[1]	[2–6]		[1]	[7, 8]				[9]		

* EEd = Electrostatic Embedding with Electron Density, EEq = Electrostatic Embedding with Atomic Charges, ME = Mechanical Embedding

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