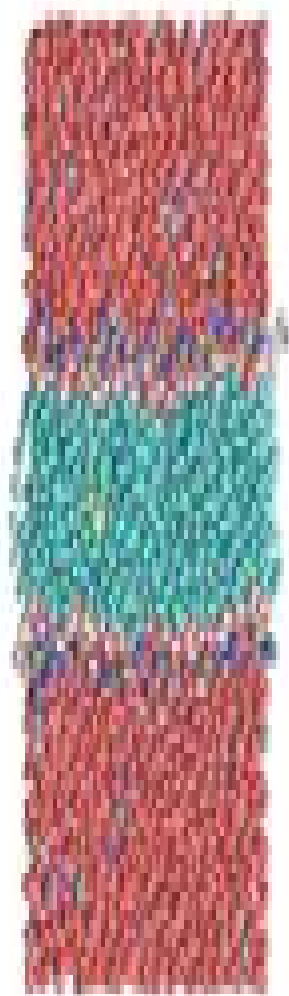


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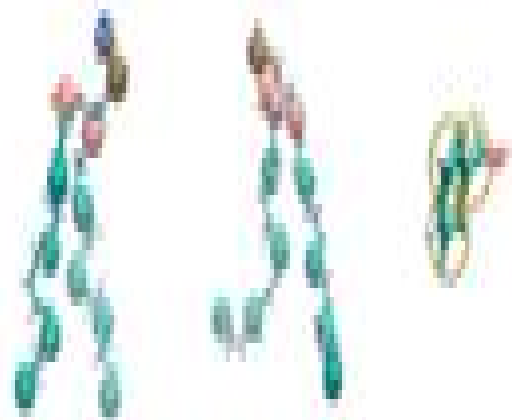


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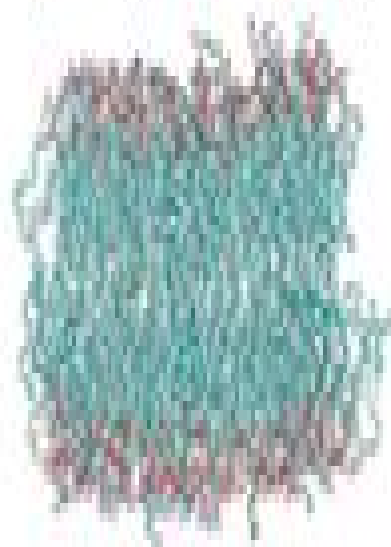
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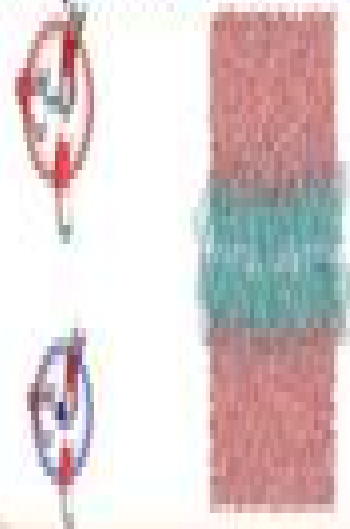
Step 2: Position restrained EM and MD



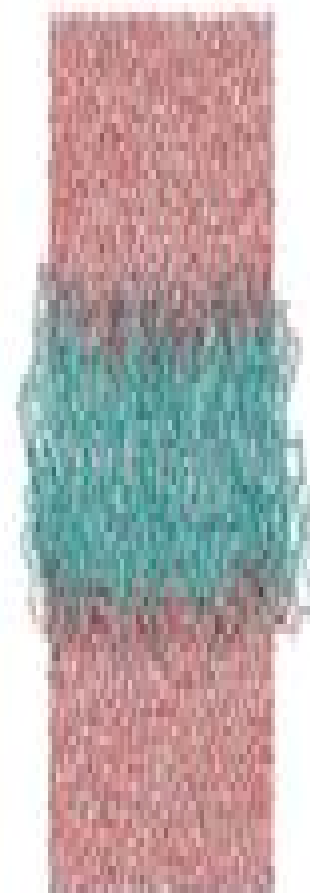
Step 3: System assembly



Step 4: Place water and ions



Step 5: EM and MD



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