

Supporting Information

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Functionalized Carbon Nanotubes as Advanced Adsorbents: Molecular Dynamics Simulation

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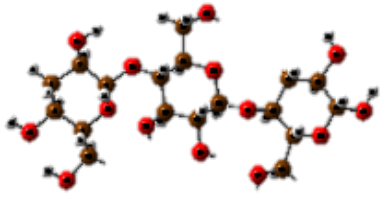
نانولوله های کربنی عاملدار شده به عنوان جاذب های پیشرفته:
شبیه سازی دینامیک مولکولی

شعله اعلائی¹ (<https://orcid.org/0000-0003-4266-596X>)

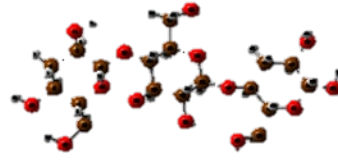
¹گروه فیزیک، واحد ارومیه، دانشگاه آزاد اسلامی، ارومیه، ایران

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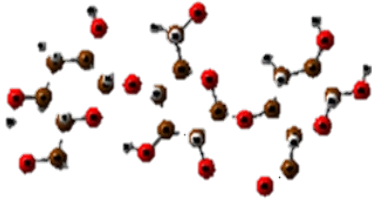
شکل S1. پیکر بندی های مختلف بهینه سازی شده از سل-تری اوز



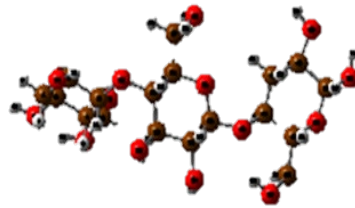
Cel-1



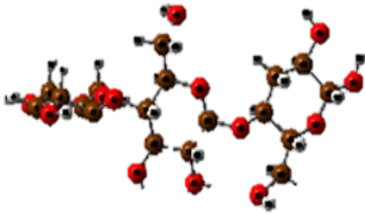
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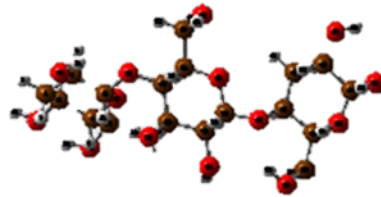
Cel-3



Cel-4

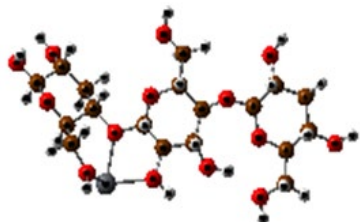


Cel-5

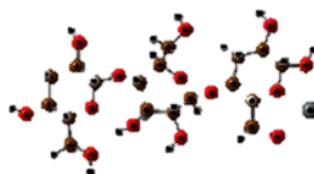


Cel-6

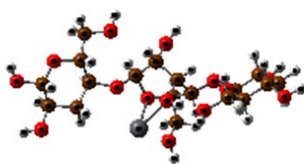
شکل S2. شکل هندسی و پیکر بندی های بهینه شده و اختلاف انرژی آنها به پایدار ترین پیکر بندی



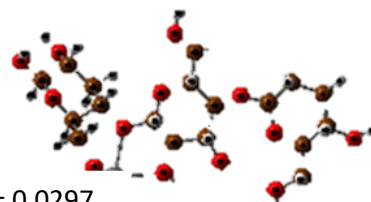
cel-pb1=0.0464



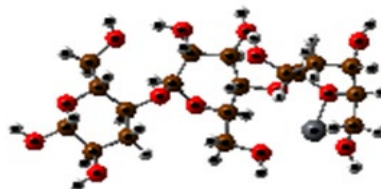
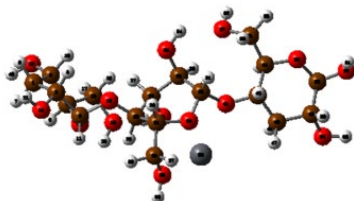
cel-pb2=0.1227



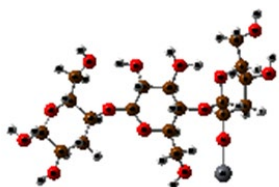
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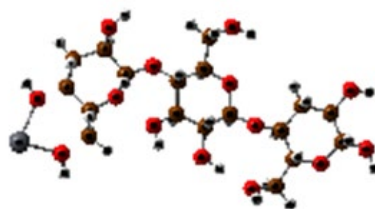
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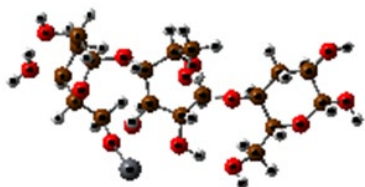
cel-Pb5=0



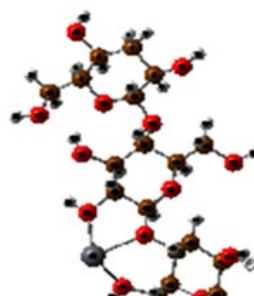
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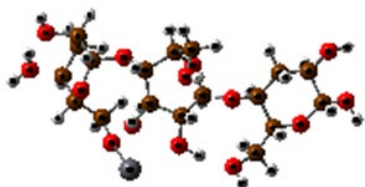
cel-Pb7= 0.0102



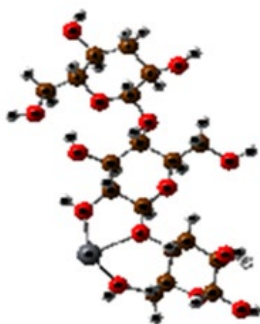
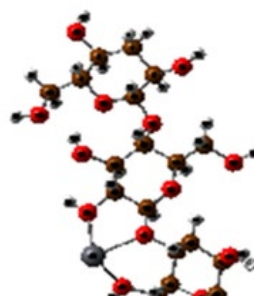
cel-Pb8= 0.0463



cel-Pb9=0.0970



cel-Pb10= 0.0110



cel-Pb11=0.0029