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Ab initio Investigation of Cu Nanoparticle Behavior Under High Electric Field

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Metal surfaces have inevitable defects, such as dust particles, scratches, and protrusions caused by manufacture. Such defects will generate local electric field enhancement, occur vacuum breakdown, give rise to great damage to metal devices. The Compact Linear Collider (CLIC) in CERN, is one of the important examples where vacuum breakdown may affect the performance efficiency of the entire machine. Based on this, it is necessary to investigate how high electric field affect metal surfaces. In this work, Cu, as a common cathodes material, is chosen to study its behavior under high electric field.

In our preliminary estimates, when increase the bond length between Cu pair and scan its total energy, we obtain a total energy curve with a potential well. Then the same process is operated under electric field, it is observed that the potential well disappeared. After that, external electric field also be added in Cu cell, it can be seen clearly that the surface bend because of the electric fields. Such phenomenon demonstrates that electric field affects the behaviour of Cu nanoparticles, and need to go deeper in further studies.

Topic

Modeling and Simulations

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