Orientation and heat capacity of horizontally adsorbed molecules in electric fields

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The orientation and heat capacity of horizontally adsorbed molecules are investigated in static electric fields. The energy spectrum and wave functions are evaluated to probe the rotational characteristics of the molecule. Numerical results indicate that the electric field and quantum confinement effect lead to anticrossing behavior in the energy levels. The orientation reveals a step feature due to the two anticrossings in the ground state. Moreover, the heat capacity displays multiple peaks near the anticrossings. By comparison, each peak of heat capacity corresponds to a particular degree of orientation.