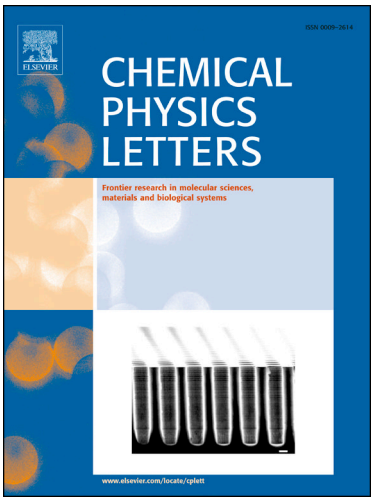

Unusual chemical bonding in the beryllium dimer and its twelve vibrational levels

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Unusual chemical bonding in the beryllium dimer and its twelve vibrational levels

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Abstract

The ab initio calculations have shown that the atoms in the beryllium dimer are covalently bound at the low-lying vibrational energy levels with ν=0-4, while at the higher levels with ν=5-11 the atoms are bonded by the van der Waals forces near the right turning points. The developed ab initio modified EMO potential function, in distinction with the original EMO function, which was used for a description of the experimental vibrational levels, not only has the correct dissociation energy, but also describes all twelve vibrational energy levels with a smaller RMS error of less than 0.4 cm^{-1}.

Keywords: covalent bonding, van der Waals bonding, vibrational energy levels, beryllium dimer

1. Introduction

The latest spectral experiment reported in [1] has caused a new wave of research in the beryllium dimer, because it has become the first many-electrons molecule for which almost all vibrational energy levels are experimentally detected. Thus, theoreticians got an excellent example for testing the many-

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