Ab initio molecular orbital calculations of octahedral silicate cluster

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In order to understand the 6-folded Si-O bond nature from the view point of the electric state, ab initio molecular orbital calculation has been carried out. One of the pauling-baur rule that the shared edge is shorter than the unshared is proved by the present calculation. It is supposed that the shortening of shared edge with compression involves the increase of covalency therein.