Geometry optimization and charge density distribution of single layer of Zn-based metal-organic framework

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The set of theoretical approaches were used to obtain the optimized geometries, electronic structure and charge density of single layer of metal-organic framework based on $Zn[Zn_2(TBAPy)(H_2O)_2\,3.5DEF]n$(MOF-Zn). Infinite monolayer composed of the unit cell of the MOF-Zn was considered. Ground state properties were researched using density functional theory with BLYP and PBE exchange-correlation functionals. The influence of the type of these approaches on the spatial structure and charge density was discussed.