Structural stability and initial decomposition mechanisms of BTF crystal induced by vacancy defects: a computational study

Jincheng Ji, Weihua Zhu*

Institute for Computation in Molecular and Materials Science, School of Chemistry and Chemical Engineering, Nanjing University of Science and Technology, Nanjing 210094, China

E-mail: zhuwh@njust.edu.cn
Fig. S1 RDFs of N-O, C-N and C-C atomic pairs of the V1 system at different times.
Fig. S2 RDFs of N-O, C-N and C-C atomic pairs of the V2-1 system at different times.
Fig. S3 RDFs of the N-O, C-N and C-C atomic pairs of the V3-1 system at different times.