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

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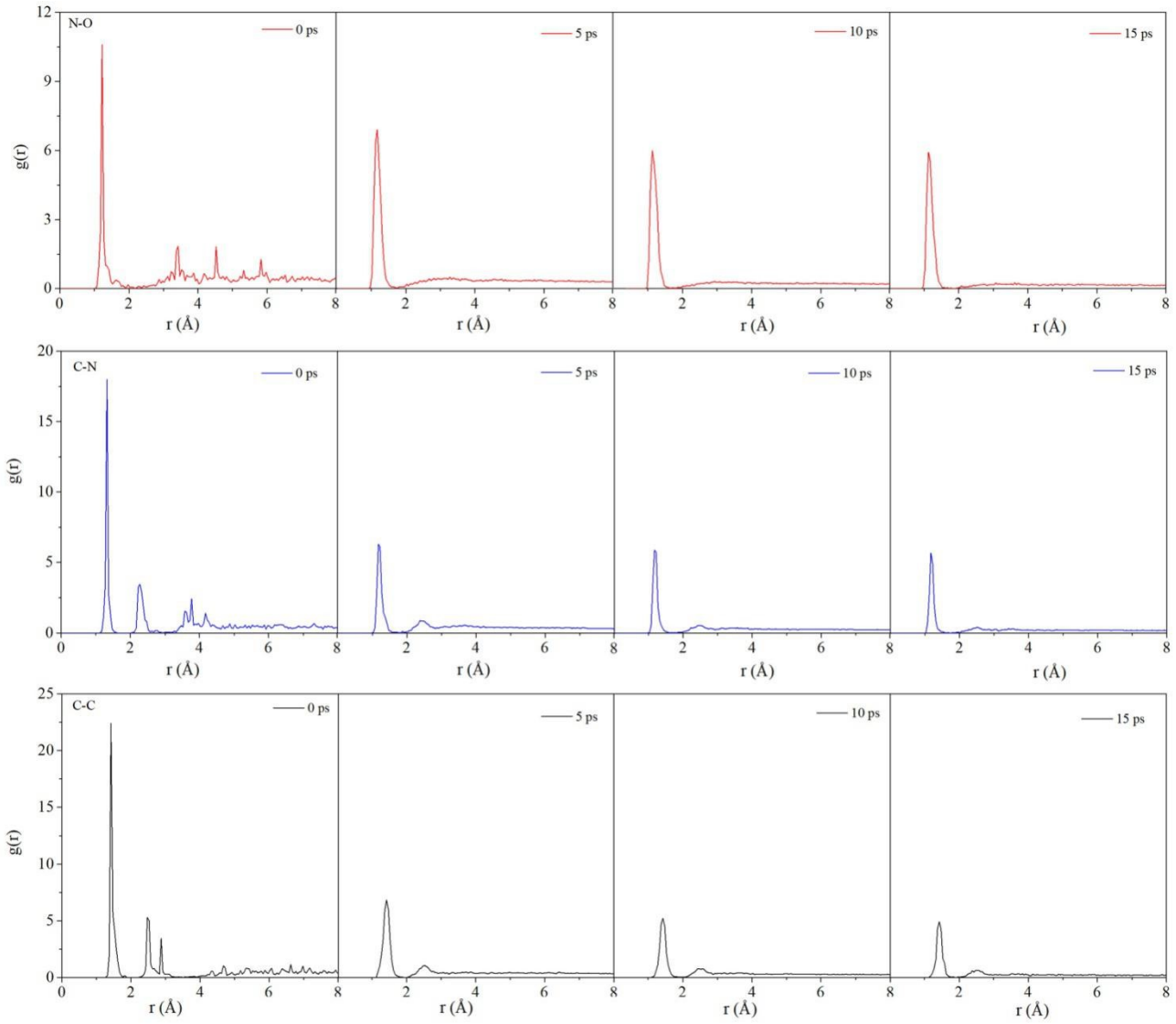

Fig. S1 RDFs of N-O, C-N and C-C atomic pairs of the V1 system at different times.

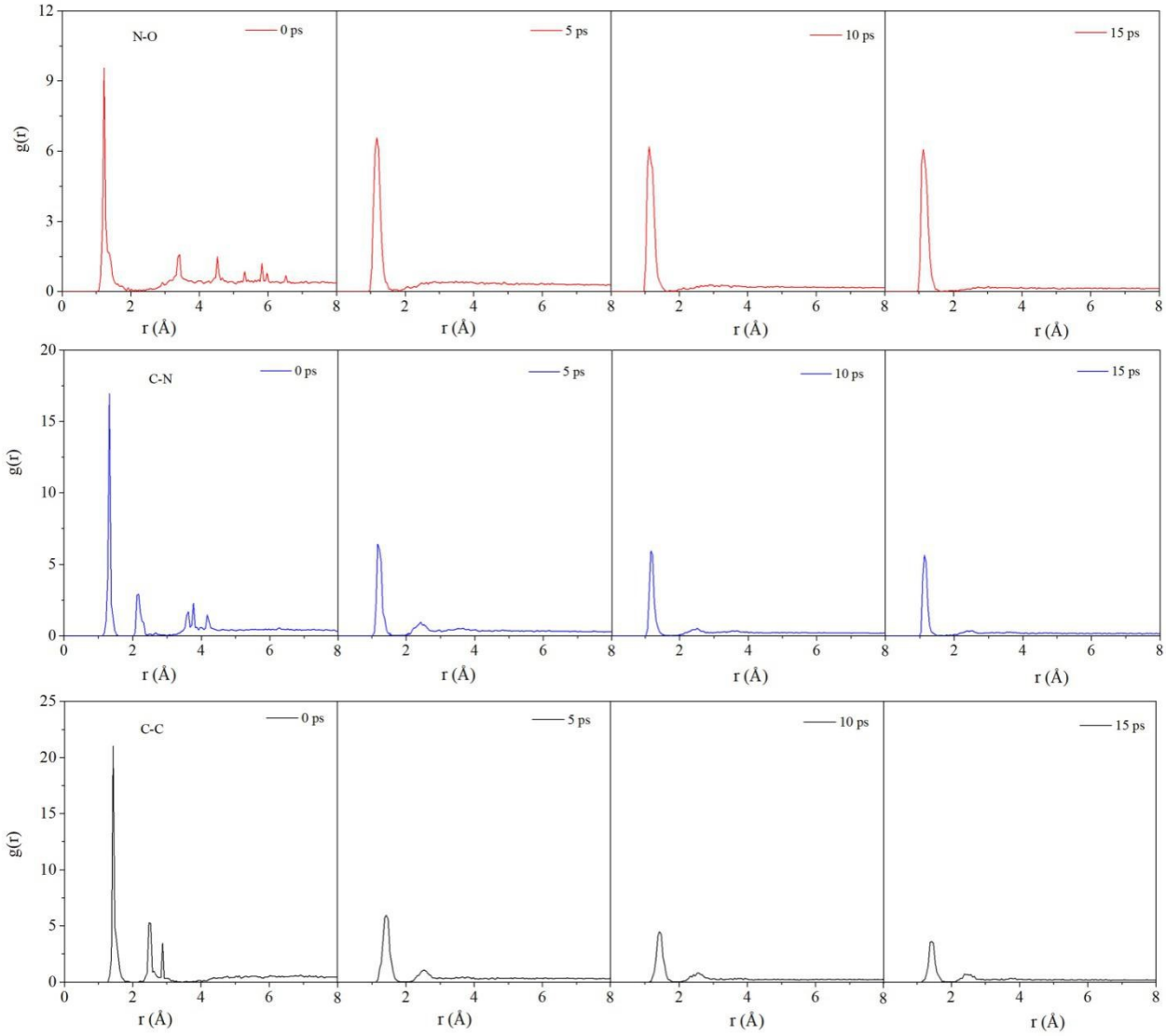

Fig. S2 RDFs of N-O, C-N and C-C atomic pairs of the V2-1 system at different times.

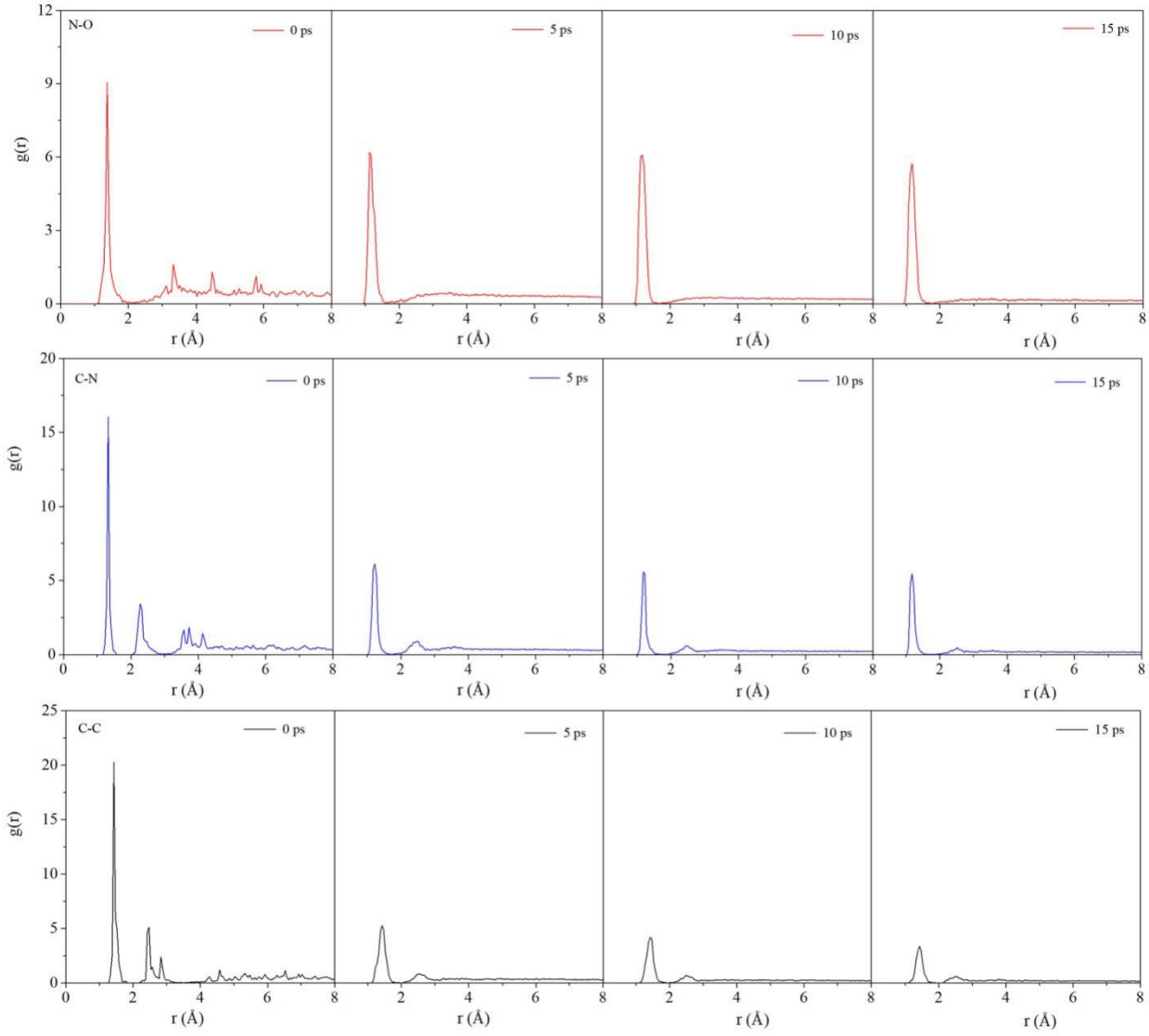

Fig. S3 RDFs of the N-O, C-N and C-C atomic pairs of the V3-1 system at different times.