

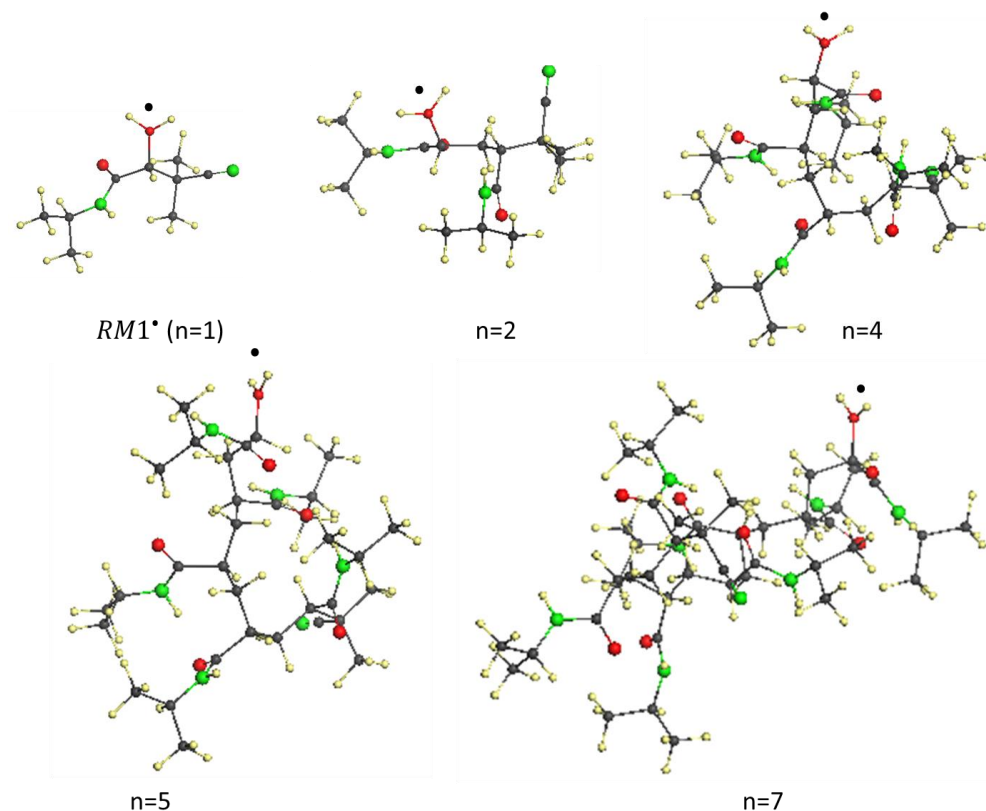
# Virtual Free-Radical Polymerization of Vinyl Monomers in View of Digital Twins

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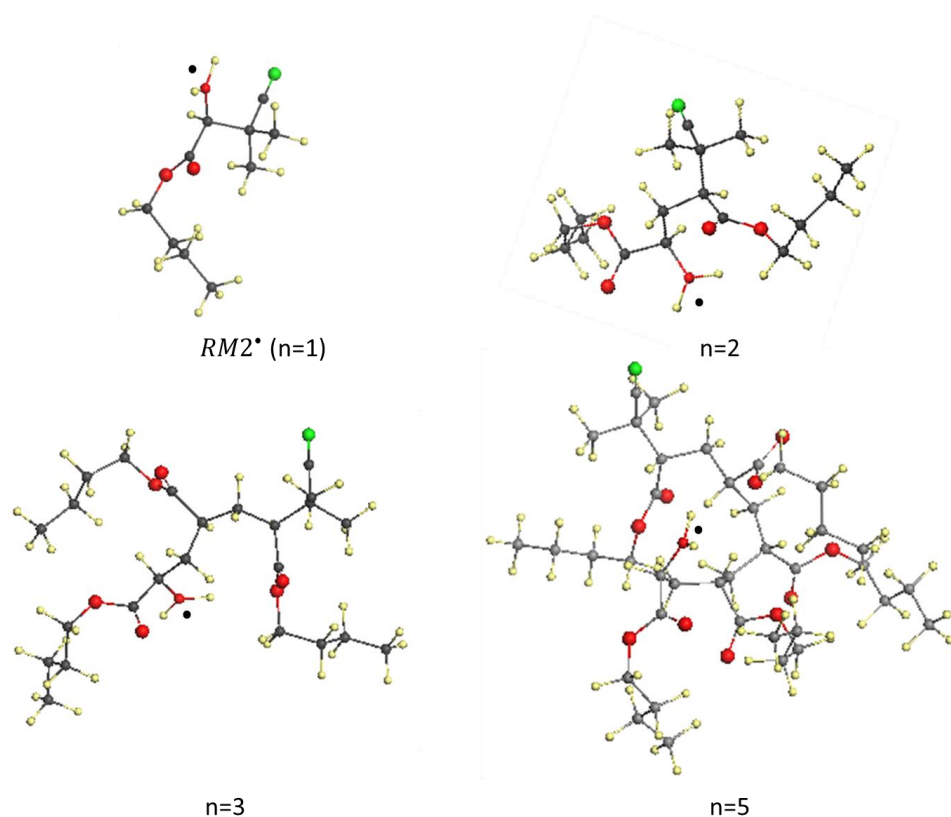
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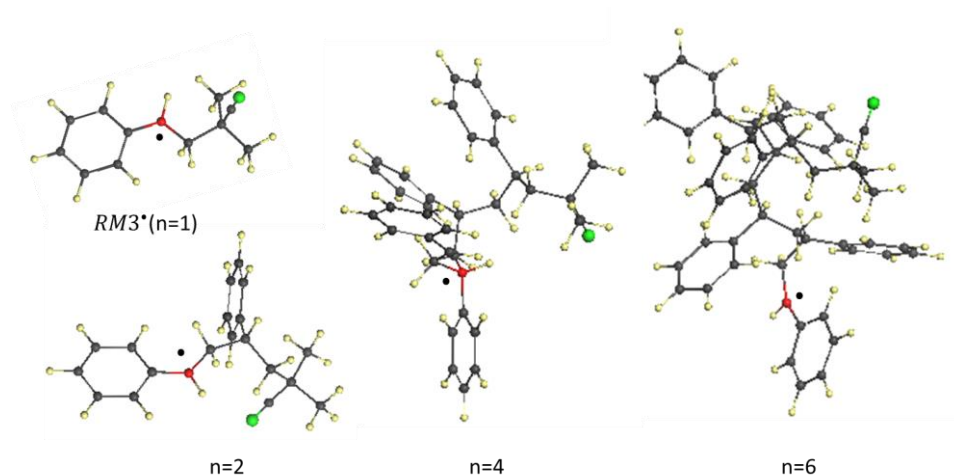
## SUPPORTING MATERIALS



**Figure S1.** Equilibrium structures of oligomer radicals  $R(M1)_n^\bullet$  for  $n= 1, 2, 4, 5$  and  $7$ . Small yellow, gray and red balls mark hydrogen, common and target carbon atoms, respectively. The latter are additionally indicated by small black balls. Larger green and red balls depict nitrogen and oxygen atoms. UHF AM1 calculations.



**Figure S2.** Equilibrium structures of oligomer radicals  $R(M2)_n^\bullet$  for  $n=1, 2, 3$  and  $5$ . Small yellow, gray and red balls mark hydrogen, common and target carbon atoms, respectively. The latter are additionally indicated by small black balls. Larger green and red balls depict nitrogen and oxygen atoms. UHF AM1 calculations.



**Figure S3.** Equilibrium structures of oligomer radicals  $R(M3)_n^\bullet$  for  $n=1, 2, 4$ , and  $6$ . Small yellow, gray and red balls mark hydrogen, common and target carbon atoms, respectively. The latter are additionally indicated by small black balls. Larger green balls depict nitrogen atoms. UHF AM1 calculations.