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Oxidation of Cu and surface activity study of CuO using ReaxFF molecular dynamics during short-pulsed laser irradiation of suspension

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Laser irradiation of nano-particles (LINP) suspended in a solvent has been recently introduced as a suitable method for the production of complicated sub-micron particles. Mostly, various nano-particles suspended in a solvent are irradiated with a short-pulse laser. The reactions taking place on the surface of particles are not exactly those which are predicted by classical thermodynamics because the process is too fast and mostly there would not be any equilibrium condition. The main concern of this study is to investigate the possible chemical reactions containing bond breakings and bond formations which are studied by reactive bond force field theory (ReaxFF) in Cu-O system during LINP. This work was supported by the Polish National Science Center Program No. 2018/31/B/ST8/03043.

