Fig. 16. Polyaniline production with a laccase double mutant (DM). A. Formula of conductive polyaniline. B. Two mutations predicted by PELE simulations enabled efficient electron transfer (estimated by QM/MM calculations) from docked aniline (CPK-colored spheres) to laccase copper-1 (cyan spheres) in DM (right) compared with parental laccase (left). C. Experimental demonstration of faster polyaniline production (left) and darker color (right) by DM compared with parental laccase. Adapted from Santiago et al. (2016).