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Evaluating cellulose potential for estrogen micropollutants removal from water effluents using quantum chemical modeling and calculations

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1 **Evaluating cellulose potential for estrogen micropollutants removal from**  
2 **water effluents using quantum chemical modeling and calculations**

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10 **Abstract**

11 This paper is devoted to investigate the suitability of cellulose for estrogens micropollutants  
12 removal from water effluent. For this purpose, the sorption of eight estrogens including  
13 Estradiol, Estrone, Testosterone, Progesterone, Estriol, Mestranol, Ethinylestradiol and  
14 Diethylstilbestrol were investigated. The charge density profiles and sorption curves were  
15 obtained and discussed using quantum chemical calculations where the Accelrys Materials  
16 Studio software and COSMO-SAC model were employed. The geometry optimization of  
17 compound molecule and energy minimizations was performed using the Dmol3 Module and  
18 density functional theory of generalized gradient approximate and Volsko-Wilk-Nusair  
19 functional. We found that cellulose cannot be a reliable choice of sorbent for removal of  
20 Estrone and Estradiol, but it is a poor choice of sorbent for removal of Estriol,  
21 Ethinylestradiol. Cellulose can be used for Diethylstilbestrol, Mestranol, Testosterone and  
22 Progesterone removal from estrogens containing effluents.

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