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First-principles theory of coloration of WO_3 upon charge insertion[1] YU XUE, PEIHONG ZHANG, Department of Physics, University at Buffalo, State University of New York, Buffalo, NY 14260, USA — Tungsten trioxide is one of the most extensively studied electrochromic materials. Here we report density functional theory (DFT) investigations of the coloration mechanism of WO_3 upon charge insertion. Our results explains very well the systematic change in color of Na_xWO_3 from blue to golden-yellow with increasing sodium concentration. We find that proper accounts for the free-carriers contribution to the optical response are critical for a quantitative understanding of the coloration mechanism in this system. We thank Dr. Yong Zhang for his helpful discussion. We thank Dr. M. D. Jones for his assistance in coding. We acknowledge the computational support provided by the Center for Computational Research at the University at Buffalo, SUNY.

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