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First-principles theory of capacitive and electrochemical energy storage JOONGOO KANG, YONG-HYUN KIM, National Renewable Energy Laboratory, Golden, CO 80401 — Recently there has been much interest in development of new electrochemical capacitors to meet high-power and high-energy applications. Pseudo-capacitors using fast surface redox reactions can store electrical energy of 10 to 100 times larger than supercapacitors and still exhibit fast and reversible charge-discharge responses in contrast to batteries. Yet, energy storage mechanisms in super- and pseudo-capacitors have not been fully understood at the level of electrons. Here we have performed first-principles calculations for electrical double layers of a TiO_2 (101) electrode and solvated lithium ions on the surface, with the ethylene carbonates (EC) as solvent molecules. As Li ions are desolvated from Li-EC_4 to Li-EC_3 and bare Li ions, the capacitance gets larger due to the reduced distance between the Li ions and the electrode. When Li ions are intercalated into the subsurface of the TiO_2 electrode as supposed in pseudocapacitors, the electrostatic energy due to charge separation is reduced for a given stored charge, but the electrochemical reaction starts to occur causing a large increase in the capacitance.

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