Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

DYNAMICAL CORRECTION OF THERMOELECTRIC COEFFICIENTS FOR STRONGLY INTERACTING ELECTRONS IN THE COULOMB BLOCKADE REGIME KAIKE YANG, Universidad del Pais Vasco, San Sebastian, Spain — FOR MOLECULES WEAKLY COUPLED TO LEADS THE EXACT ZERO-BIAS KOHN-SHAM CONDUCTANCE CAN BE ORDERS OF MAGNITUDE LARGER THAN THE TRUE CONDUCTANCE DUE TO THE LACK OF DYNAMICAL EXCHANGE-CORRELATION (XC) EFFECTS. RECENTLY, IT HAS BEEN SHOWN [1] HOW THESE DYNAMICAL XC CORRECTIONS CAN BE CALCULATED USING ONLY QUANTITIES OBTAINED FROM STATIC DENSITY FUNCTIONAL THEORY. HERE, WE INVESTIGATE THE THERMOELECTRIC TRANSPORT AND DERIVE THE XC CORRECTION TO THE SEEBECK COEFFICIENT. WE FIND THAT THE DYNAMICAL CORRECTION TO THE SEEBECK COEFFICIENT IS DETERMINANT IN EVALUATING THE THERMOPOWER: THE ABSOLUTE VALUE OF THE DYNAMICAL CORRECTION FOR THE SEEBECK COEFFICIENT IS, FOR CERTAIN VALUES OF GATE VOLTAGE, MUCH LARGER THAN THAT OF THE KOHN-SHAM TERM. FINALLY, WE COMPARE OUR DENSITY FUNCTIONAL CALCULATIONS TO THE RATE EQUATION [2] AND THE EXPERIMENTAL RESULTS [3]. [1] S. KURTH, ET AL., PRL , 030601 (2013). [2] C. W. J. BEENAKKER, ET AL., PRB , 9667 (1992). [3] J. P. SMALL, ET AL., PRL , 256801 (2003).

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Date submitted: 08 Nov 2015 Electronic form version 1.4