Atomic-scale Field-effect Transistor as a Thermoelectric Power Generator and Self-powered Device.

Yu-Shen Liu, Hsuan-Te Yao, and Yu-Chang Chen*

Department of Electrophysics, National Chiao Tung University, 1001 Ta Hush Road, Hsinchu 30010, Taiwan

Using first-principles approaches, we have investigated the thermoelectric properties and the energy conversion efficiency of the paired metal-Br-Al junction. Owing to the narrow states in the vicinity of the chemical potential, the nanojunction has large Seebeck coefficients such that it can be considered an efficient thermoelectric power generator. We also consider the nanojunction in a three-terminal geometry, where the current, voltage, power, and efficiency can be efficiently modulated by the gate voltages. Such current-voltage characteristics could be useful in the design of nano-scale electronic devices such, as a transistor or switch. Notably, the nanojunction as a transistor with a fixed finite temperature difference between electrodes can power itself using the Seebeck effect.

I. INTRODUCTION

In the past decade, considerable concern has arisen regarding the transport properties of atomic-scale junctions, which are the basic building blocks for molecular electronics[1,2]. This concern is motivated by the aspiration to develop new forms of electronic devices based on subminiature structures and by the desire to understand the fundamental properties of electron transport under non-equilibrium[3]. A growing number of research studies are now available to diversify the scope of electron transport properties in molecular/atomic junctions, including current-voltage characteristics[4–6], inelastic electron tunneling spectroscopy (IETS)[7–16], shot noise[17–20], counting statistics[21], local heating[22,23], and gate-controlled effects[24–28]. Substantial progress in experiment and theory has been achieved[29–31].

Recently, growing attention has been paid to the thermopower of nanojunctions. Pioneering experiments have been conducted to measure the Seebeck coefficients at the atomic and molecular level[32–35]. The Seebeck coefficient is related not only to the magnitude, but also to the slope of the transmission function in the vicinity of chemical potentials. Thus, it can provide richer information than the current-voltage characteristics regarding the electronic structures of the molecule bridging the electrodes[36]. The thermoelectric effect hybridizes the electron and energy transport, which complicates the fundamental understanding for quantum transport of electron and energy under non-equilibrium conditions. This has spurred rapid developments in the fundamental thermoelectric theory in nanojunctions[37–47] including the effects of electron-vibration interactions [48–50]. The Seebeck coefficient is typically measured under equilibrium condition, non-equilibrium current and inelastic effects potentially offer new possibilities of engineering systems leading to enhanced the thermopower[51,52]. The emergence of thermoelectric nanojunctions may also have profound implications on the design of subminiature energy-conversion devices, such as nano-refrigerators[53–55].

Thermoelectric power generators in bulk systems employ electron gas as a working fluid. It directly converts thermal energy into electric energy using the Seebeck effect. Provided a temperature difference is maintained across the device, it can generate electric power converted from the thermal energy. In this paper, we explore the energy conversion mechanism of nanojunctions. We present a parameter-free first-principles calculations for a thermoelectric power generator in a truly atomic-scale system. To gain further insight into the mechanism of energy conversion, we also developed an analytical theory for it. As a specific example, we consider an atomic junction depicted in Fig. 1(a), where the left and right electrodes serve as independent cold- and hot-temperature reservoirs, respectively. This is not just an academic example since recent studies have demonstrated the capability to assemble one magnetic atom on a thin layer of atoms on the surface of STM[56]. A similar technique might be applicable to a single Al atom adsorbed onto a layer of Br atoms on the metal surface. In this regard, the atomic junction could be formed by bringing two identical pieces of metal-Br-Al surfaces close together before the reconstruction of Br and Al atoms occurs.

As it was found in Ref. 57, the paired metal-Br-Al junction shows interesting device properties, such as negative differential resistance, that utilize the relatively narrow density of states (DOSs) near the chemical potentials. The narrow DOSs are due to the weak coupling between the Al atoms and the electrodes via the "spacer" Br atoms[58,59]. This junction also serves as an efficient field-effect transistor because the narrow DOSs near chemical potentials can be easily shifted by the gate voltages. As the Seebeck coefficients are relevant to the slope of DOSs, the sharp DOSs result in a large magnitude in the Seebeck coefficient[52]. When a temperature difference is maintained between electrodes in a closed circuit, the Seebeck effect generates an electromotive force (emf), which drives a current flowing through the junction, hence the nanojunction can also be considered as an efficient thermoelectric power generator[60].

We investigate further the possibility of powering an atomic-scale device as a field-effect transistor using heat instead of electricity. To illustrate this point, we consider the paired metal-Br-Al junction in a three-terminal geometry. When a finite temperature difference is maintained between electrodes, the Seebeck effect converts the