



# Molecular dynamics simulation of the interfacial thermal resistance between phosphorene and silicon substrate



Jingchao Zhang<sup>a</sup>, Yang Hong<sup>b</sup>, Mengqi Liu<sup>c</sup>, Yanan Yue<sup>d</sup>, Qingang Xiong<sup>e,\*</sup>, Giulio Lorenzini<sup>f,\*</sup>

<sup>a</sup> Holland Computing Center, University of Nebraska-Lincoln, Lincoln, NE, 68588, USA

<sup>b</sup> Department of Chemistry, University of Nebraska-Lincoln, Lincoln, NE 68588, USA

<sup>c</sup> T-Rex Engineering + Construction, Houston, TX 77015, USA

<sup>d</sup> School of Power and Mechanical Engineering, Wuhan University, Wuhan, Hubei 430072, China

<sup>e</sup> Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

<sup>f</sup> Department of Industrial Engineering, University of Parma, 43124 Parma, Italy

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## ABSTRACT

Phosphorene is a recently discovered member of the two-dimensional (2D) monolayer materials, which has been reported to exhibit unique characteristics on mechanical and thermal properties. This study is the first time to show the exceptional thermal conductance between phosphorene and crystalline silicon substrate through classical molecular dynamics (MD) simulations. MD simulations revealed that under conventional conditions, the interfacial thermal resistance ( $R$ ) between phosphorene and silicon is very low and independent on the thickness ( $h$ ) of silicon substrate when  $h$  is larger than 3.12 nm. It was also found that  $R$  decreases remarkably with the increases in system temperature ( $T_{ie}$ ) and contact strength ( $\chi$ ). To further explicitly display the superiority of phosphorene on interfacial heat transfer,  $R$  of other two popular 2D monolayer materials, *i.e.*, graphene and silicene, were calculated for comparison. The comparisons revealed that  $R$  of phosphorene shows two distinct advantages over graphene and silicene. On one hand, within the studied ranges of  $T_{ie}$  and  $\chi$ ,  $R$  between phosphorene and silicon substrate is about quarter of that between graphene and silicon substrate, which proves that phosphorene is really a high-performance 2D monolayer material for interfacial heat transfer. On the other hand, with the increases in  $T_{ie}$  and  $\chi$ ,  $R$  between phosphorene and silicon substrate decreases more sharply than that between silicene and silicon substrate, indicating that phosphorene is more sensitive to environmental variations.

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## 1. Introduction

The novel structure that monolayer atoms are aligned with honeycomb lattice has brought two-dimensional (2D) materials such as graphene and silicene many distinguished thermo-physical properties compared to traditional materials. One of the remarkable properties these 2D monolayer materials possess is their rather low interfacial thermal resistance for heat dissipation into adjacent substrates, which makes them as appealing candidates for the design of next-generation nano-devices [1–5]. Phosphorene, a newly synthesized 2D monolayer material, has attracted great interest in recent years due to its novel structural and electronic properties, *e.g.*, layer-dependent direct bandgaps and high electron/hole mobility [6–8]. It has been reported that

phosphorene-based field-effect transistors exhibit very high carrier mobility and extraordinary on/off ratios [9–11], which show its great potential to be applied to high-performance nano-electronic devices. However, whether phosphorene is also outstanding on interfacial heat transfer still remains unclear.

Because of the extremely small spatiotemporal scales, existing experimental approaches still face inherent challenges in accurate measurement of thermal properties for 2D monolayer materials, including interfacial thermal resistance. In recent years, with the dramatic increases in computational power, classical molecular dynamics (MD) simulation which directly resolves thermal properties at atomistic scale, has been widely used in the investigation of 2D monolayer materials. Thermal conductivity, thermal rectification as well as interfacial thermal resistance of 2D monolayer materials, have been extensively studied by MD simulations [12–17]. These MD simulations, to a large extent, complement experimental approaches to quantitatively clarify the novel thermal properties of 2D monolayer materials, especially those of graphene

\* Corresponding authors.

E-mail addresses: [qgxiong@126.com](mailto:qgxiong@126.com) (Q. Xiong), [giulio.lorenzini@unipr.it](mailto:giulio.lorenzini@unipr.it) (G. Lorenzini).

## Nomenclature

$E$	three body system energy	$R$	interfacial thermal resistance
$f_c$	cutoff function	$E_t$	phosphorene system energy at time $t$
$f_R$	repulsive pair potential	$E_0$	phosphorene initial system energy before heating
$f_A$	attractive pair potential	$q_{in}$	thermal impulse energy
$r_{ij}$	interatomic distance between atoms $i$ and $j$	$t$	time step
$b_{ij}$	monotonically decreasing function of the coordination of atoms $i$ and $j$	$h$	substrate thickness
$V_2$	two-body bond stretching energy	$\omega$	phonon frequency
$V_3$	three-body angle bending interactions energy	$G(\omega)$	phonon power spectrum
$A, K$	energy parameter	$A(\omega)$	overlap area
$\chi$	coupling strength	$\delta$	phonon power spectra overall factor
$T_P$	temperature of phosphorene	$B, \rho_1, \rho_2, \theta, \theta_0$	geometry parameters
$T_{Si}$	temperature of silicon top layers	$r_{max}, r_{max12}, r_{max13}$	cutoff distances
$T_{ie}$	initial equilibrium temperature	$\varepsilon_{P-Si}, \varepsilon_{C-Si}, \varepsilon_{Si-Si}$	potential well depth
		$\sigma_{P-Si}, \sigma_{C-Si}, \sigma_{Si-Si}$	potential zero point distance

and silicene. These MD studies have contributed significantly to our knowledge on the thermal behaviors of 2D materials, ranging from fundamental to application levels.

So far, to the best of our knowledge, MD simulations of interfacial thermal resistance for 2D monolayer materials have not been applied to phosphorene. This is majorly because compared with other 2D monolayer materials, until recently the key parameters to quantitatively determine interactions among atoms within phosphorene, such as cut-off distances and bonding angles, have not been available. The lack of such key parameters has largely hindered the utilization of the powerful MD technology to study the interfacial thermal resistance of phosphorene. Very recently, using the valence force field model [18], Wu accurately determined those parameters required by the Stillinger–Weber (SW) potential [19]. Those first-principle calculated parameters have been proved to be accurate when applied to model the mechanical properties [20,21] and thermal conductivity of phosphorene [22,23] and phosphorus nanotubes [24]. Therefore, the way to successful MD simulation of the interfacial thermal resistance for phosphorene has been paved by those precise first-principle calculated parameters.

In most nano-devices, silicon is used as substrate to support 2D monolayer materials for heat dissipation. Therefore, it is highly desirable to characterize the interfacial heat transfer between phosphorene and silicon. This study explored the interfacial thermal resistance between phosphorene and crystalline silicon substrate by MD simulations with the SW potential using the foregoing mentioned precise first-principle calculated parameters. A transient pump–probe technique mimicking the experimental thermo-reflectance method was applied to evaluate the interfacial thermal resistance. To comprehensively demonstrate the characteristics of the interfacial thermal resistance between phosphorene and silicon substrate, cases with graphene and silicene contacting silicon substrate were also included for comparison. In the following, the physical models and computational setup are first described. Then, the characteristics of interfacial thermal resistance between phosphorene and silicon substrate are presented. The effects of substrate thickness, system temperature and coupling strength on the interfacial thermal resistance are explored. Finally, the superiority of phosphorene on interfacial thermal resistance compared to graphene and silicene is discussed.

## 2. Numerical models

In a typical MD simulation, the most important aspect is to have an appropriate inter-atom potential. It should be not only physi-

cally accurate but also computationally economic. In this study, the classical Tersoff potential was chosen to model the interactions among silicon atoms [25] as

$$E = \frac{1}{2} \sum_i \sum_{j \neq i} f_c(r_{ij}) [f_R(r_{ij}) + b_{ij} f_A(r_{ij})], \quad (1)$$

where  $E$  is the three-body system energy, and  $f_c(r_{ij})$  is the cutoff function to limit the range of the potential since the short-range interaction can save great computational effort. The function  $f_R(r_{ij})$  represents the repulsive pair potential, which includes the orthogonalization energy when atomic wave functions overlap, and  $f_A(r_{ij})$  is an attractive pair potential associated with bonding. The  $b_{ij}$  term is a monotonically decreasing function of the coordination of atoms  $i$  and  $j$ . Detailed information on classical Tersoff potential can be found in Ref. [25]. It has been proved by many prior MD studies that the micro-scale behaviors for silicon can be successfully reproduced by the classical Tersoff potential [26–28]. As mentioned above, the interactions among phosphorene atoms were modeled by the SW potential as follows

$$V_2 = A e^{\left[ \frac{\rho}{r - r_{max}} \right]} \left( \frac{B}{r^4} - 1 \right), \quad (2)$$

$$V_3 = K e^{\left[ \frac{\rho_1}{r_{12} - r_{max12}} + \frac{\rho_2}{r_{13} - r_{max13}} \right]} (\cos \theta - \cos \theta_0)^2, \quad (3)$$

where  $V_2$  and  $V_3$  represent the two-body bond stretching and three-body angle bending interactions respectively.  $A$  and  $K$  the energy parameters and  $B, \rho_1, \rho_2, \theta$  and  $\theta_0$  are the geometry parameters. These parameters were calculated by the first-principle valence force field model [18]. The cutoff distances  $r_{max}, r_{max12}$  and  $r_{max13}$  are determined by the lattice structures. Following our previous simulations [29], the coupling between silicon and phosphorene was modeled by the classical 12-6 Lennard–Jones potential as

$$V(r) = 4\chi \varepsilon_{P-Si} \left[ \left( \frac{\sigma_{P-Si}}{r} \right)^{12} - \left( \frac{\sigma_{P-Si}}{r} \right)^6 \right], \quad (4)$$

where  $r$  is the distance between silicon and phosphorene atoms.  $\varepsilon_{P-Si}, \sigma_{P-Si}$ , and  $\chi$  are the depth of the potential well (eV), zero potential distance (Å), and coupling strength, respectively. It is worth noting that another popular approach to manipulate the coupling strength is to insert an interlayer at the interfaces [30–32]. In this study, the values of  $\varepsilon_{P-Si}$  and  $\sigma_{P-Si}$  were determined by the universal force field model [33], resulting in  $\varepsilon_{P-Si} = 15.205$  meV and  $\sigma_{P-Si} = 3.760$  Å. All the MD simulations in this study were performed on the LAMMPS Molecular Dynamics Simulator [34].

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