

# Phononics of graphene, layered materials, and heterostructures

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The research field of *phononics* deals with quanta of crystal lattice vibrations—phonons—whose characteristics influence the elastic, acoustic, thermal, optical, and electrical properties of materials.<sup>1–4</sup> Phononics draws an analogy with *photonics*, particularly when it comes to the use of periodic metamaterial structures for the purpose of changing the energy dispersion of the elemental excitations and inducing an energy bandgap.<sup>5,6</sup> This research field is often also termed *nano-phononics* or nanoscale *phonon engineering* to emphasize the importance of the nanoscale dimensions for modification of the phonon dispersion and density of states.<sup>1,3</sup> The *engineering* component indicates a possibility of fine-tuning the properties of materials via controlled modification of the phonon dispersion, group velocity, and density of states. One can trace the origin of the phonon engineering concept to the first proposals of the reduction in phonon thermal conductivity in semiconductor quantum wells and nanowires by spatial confinement of acoustic phonons,<sup>7,8</sup> rather than by the phonon-boundary scattering.<sup>9</sup>

Phononics of graphene, layered materials, and heterostructures is particularly interesting, allowing one to elucidate the physics of crystal lattice vibrations and engineer the phonon spectrum to achieve new functionalities. Graphene plays an important role in this research direction and provides an extra impetus to the development of phononics. Electrons are not the only elemental excitations that reveal exotic properties in graphene.<sup>10,11</sup> Optical and acoustic phonons in graphene differ substantially from those in bulk graphite and few-layer graphene.<sup>12–14</sup> Thus, Raman spectroscopy became an integral part of graphene research. It is used to determine the number of layers,<sup>13</sup> the quality and types of edges,<sup>15</sup> and the effects of perturbations,<sup>14</sup> such as electric<sup>16</sup> and magnetic fields,<sup>17–19</sup> strain,<sup>20</sup> doping,<sup>21</sup> disorder,<sup>22</sup> and functional groups.<sup>23</sup> Similarly, for layered materials, such as hexagonal boron nitride, and transition-metal dichalcogenides, Raman and

infrared spectroscopies are accurate, nondestructive approaches to determine a wide range of properties, including the number of layers and the strength of the interlayer interactions.<sup>24</sup> Acoustic phonons, which are the dominant heat carriers in many materials, demonstrate a similar sensitivity to the number of graphene layers.<sup>25–29</sup> Graphene phononics has already led to a number of practical applications in thermal management technologies.<sup>27,30</sup>

A better understanding of the physics of phonons will enable us to engineer the phonon spectrum across a wide energy range—from sub-GHz to hundreds of THz. Fine-tuning the phonon energies and dispersion is a new tool to achieve innovative device functionalities. Engineering phonon spectra by changing the thickness of layered materials, rotating atomic planes, and hetero-interfacing elastically and dielectrically dissimilar layers is a new frontier of nanotechnology. Strongly correlated phenomena in low-dimensional materials depend crucially on the specifics of phonon spectra and phonon coupling with charge carriers or charge carrier complexes. Interest in phononics and phonon engineering goes beyond fundamental science. Control of phonon dispersion and interactions is crucial for developing next-generation electronics, spintronics, and renewable energy conversion devices. This potential of phononics research motivates the present Special Topic Issue.

Phononics research builds upon interdisciplinary work by physicists, materials scientists, chemists, nanotechnologists, and electrical and mechanical engineers. Specific contributions illustrate ongoing research in the *phononics* field. Approximately half of the papers in this issue are theoretical–computational and half are experimental works. Among the computational studies, many deal with thermal transport in layered materials.<sup>31–37</sup> The topics include interfacial thermal conduction and rectification in graphene heterostructures,<sup>31</sup> the thermal conductivity of graphene allotropes,<sup>32</sup> thermal resistance in

graphene–boron-nitride heterostructures,<sup>33</sup> strain-dependent phonon hydrodynamic transport in bilayer graphene,<sup>34</sup> the effect of stress on optical phonons and thermal conductivity in monolayer layered materials (1L-LMs),<sup>35</sup> thermoelectric properties of strongly anharmonic 1L-LMs,<sup>36</sup> and thermoelectric figure of merit in 1L-LMs as a function of carrier concentration and bipolar effects.<sup>37</sup> The rest of the theoretical–computational papers addresses other issues important for phonon transport in LMs.<sup>38–40</sup> Specifically, they discuss phonon-induced exciton weak localization in 1L-semiconductors,<sup>38</sup> the physical mechanism behind atomic-size dependence of bandgap, phonon frequency, and mechanical strength in various 1L-LMs,<sup>39</sup> and phonon properties of 1L-carbon allotropes.<sup>40</sup>

The experimental reports describe phonons in new material systems or unusual properties that are affected by phonons.<sup>41–50</sup> These include studies of elemental excitations in one-dimensional van der Waals nanowires,<sup>41</sup> electron–phonon coupling at interfaces of two-dimensional organic–inorganic heterostructures determined by *in situ* Raman spectroscopy,<sup>42</sup> effects of hot phonons and thermal stress on Raman spectra of 1L-LMs,<sup>43</sup> phase-specific phononic fingerprints in piezo-response and micro-Raman imaging of LMs,<sup>44</sup> and the incoherent-to-coherent crossover in thermal transport in alloy superlattices.<sup>45</sup> Another group of experimental papers reports on the excitonic, optical, and piezoelectric properties of LMs and heterostructures that are usually affected by phonons.<sup>46–50</sup> Specifically, these discuss the photoelectric properties of layered organic–inorganic perovskites,<sup>46</sup> excitonic properties, and ultrafast dynamics in 1L-LMs with defects,<sup>47</sup> photoluminescence of exciton tuning and strain imaging in 1L-LMs,<sup>48</sup> graphene piezoresistive properties under uniaxial strain,<sup>49</sup> and mid-infrared all-optical wavelength converters based on highly nonlinear LMs.<sup>50</sup> Many experimental papers provide examples of specific practical applications of graphene, LMs, and heterostructures.

In conclusion, this Special Topic Issue presents a selection of new results associated with phononics of layered materials and heterostructures. Exciting progress in phononics and phonon engineering is happening at a rapid pace, and we anticipate that this Issue will be relevant and interesting for many researchers and students.

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## AUTHOR DECLARATIONS

### Conflict of Interest

The authors have no conflicts to disclose.

## Author Contributions

**Andrea C. Ferrari:** Conceptualization (equal); Writing – review & editing (equal). **Alexander A. Balandin:** Conceptualization (equal); Writing – original draft (equal); Writing – review & editing (equal).

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