

Erratum: Insulating moiré homobilayers lack a threefold symmetric second-harmonic generation [Phys. Rev. Materials 8, 116203 (2024)]

Luis Enrique Rosas-Hernandez, Jose Luis Cabellos, Angiolo Huamán, Bernardo Mendoza, and Salvador Barraza-Lopez 



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The symmetry assigned to the moiré structures was incorrectly identified as $p1$ in this paper due to numerical inaccuracies. In reality, these small moiré bilayers preserved their symmetries after atomistic relaxation [1]: $p321$ for twist angles of $\theta = 38.21^\circ$ and $\theta = 73.17^\circ$ and $p3$ for $\theta = 98.21^\circ$. Nevertheless, hBN moiré homobilayers can still lack a threefold symmetric second-harmonic response, as we explain next.

Twisted hBN bilayers may be prone to shift away from their ideal ground-state configuration due to thermal or quantum fluctuations. The stacking energy landscape governs the sliding: while in untwisted hBN bilayers the energy barriers are of the order of $1.24 \text{ meV}/\text{\AA}^2$ [2], in rotated bilayers the sliding barriers are drastically reduced, reaching values as low as $0.0018 \text{ meV}/\text{\AA}^2$ [3], a value much smaller than that reported in Ref. [4] for materials undergoing quantum fluctuations. This pronounced lubricity makes moiré structures an ideal platform for observing symmetry breaking. To illustrate this mechanism, Fig. 1 presents the energy landscape for small lateral displacements of $0.02 \text{ \AA}$ of the upper monolayer in the $\theta = 38.21^\circ$ moiré structure, obtained from zero-temperature DFT calculations. Depending on the displacement, the layer group can be $p1$, $c211$, or $p321$, with only the undisplaced configuration retaining threefold symmetry. A set of evenly sampled structures across this landscape is highlighted in Fig. 1 and their corresponding SHG intensities are displayed in Fig. 2. The central $p321$ -symmetric configuration (labeled 1) exhibits the expected sixfold SHG response, whereas the shifted configurations (labeled 2–7), which fall into $p1$, show broken symmetry. At nonzero temperature, we expect the bilayer to explore the non-threefold symmetric configurations. To capture the thermally induced symmetry breaking, we model the SHG response using a thermal ensemble constructed as a Boltzmann-weighted sum over structures 1–7 at $T = 300 \text{ K}$. This choice is made since the original experimental reports [5,6] do not specify an operating temperature. The resulting SHG response, shown in Fig. 2 as a dotted line within the plot of structure 1, does not exhibit sixfold symmetry.

We cannot tell the lowermost temperature at which symmetry may be restored without carrying out additional work. One thing we say without hesitation is that materials with shallow degenerate minima can become “quantum paraelastics,” a designation implying that quantum fluctuations are sufficient for a material to overcome the energy barrier [4]. Determining such a critical temperature for the moiré bilayers is beyond the scope of this paper, nevertheless.

Two additional amendments are as follows: symmetries were denoted with an uppercase P (space groups), whereas the correct notation is the lowercase p , corresponding to layer groups [1,7,8]. Second, one of the moiré structures was inadvertently

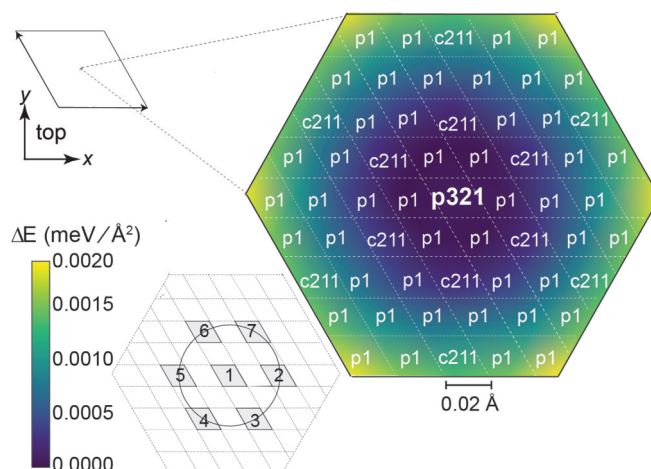


FIG. 1. Energy landscape ΔE for small lateral shifts of the upper monolayer in the moiré structure with $\theta = 38.21^\circ$. An illustration of the lateral displacements is included, where the shaded structures indicate the selected configurations for SHG calculations.

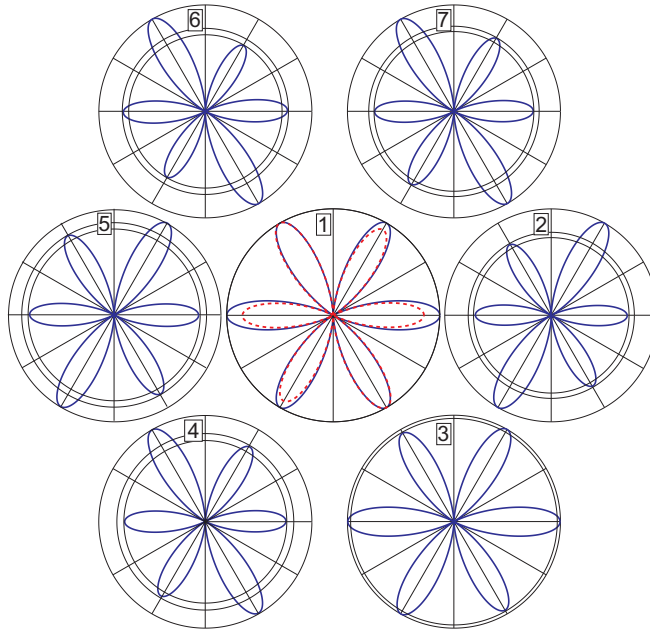


FIG. 2. SHG intensities corresponding to the shaded structures in Fig. 1. As originally stated in this paper, and although for different reasons, the SHG response of the thermal ensemble lacks threefold symmetry. This is indicated by the dotted line overlaid onto the plot of structure 1. The radial scale is the same in all plots for direct comparison.

constructed three times larger than necessary. In building the moirés, the procedure outlined by Mele [9] was followed, but a different set of primitive translations was used in this paper. Consequently, the supercell for the twist angle $\theta = 98.21^\circ$ [$(m, n) = (5, 1)$] was three times larger than required, adding unnecessary numerical effort.

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