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Insight into the structural, electronic and elastic properties of AlnQ_2 (A: K, Rb and Q: S, Se, Te) layered structures from first-principles calculations

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Highlights

- Some physical properties of AlInQ_2 (A: K, Rb and Q: S, Se, Te) are investigated
- The ground states properties compare well with the available published data
- The studied compounds are direct gap semiconductors
- The mechanical properties are investigated for the first time

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