Graph Foundation Models for Protein Electrostatics: Transfer Learning Across Ionization and Stability Prediction Tasks

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Abstract

Predicting the electrostatic properties of proteins remains a fundamental challenge for molecular biology and drug design, particularly the accurate estimation of ionization states and thermodynamic stability across diverse sequence and structural contexts. Recent breakthroughs in deep learning have opened a pathway toward graph-based foundation models that can capture complex physical interactions at scale, yet a comprehensive systems perspective that spans architecture design, transfer learning strategies, infrastructure deployment, and socio-technical implications is underdeveloped. This paper presents a long-form analysis of graph foundation models tailored for protein electrostatics, with a focus on transfer learning between the prediction of residue-level pKa values and the estimation of mutation-induced stability changes. We examine the underlying architectural trade-offs that arise when enforcing equivariance, incorporating multi-scale attention, and designing pre-training objectives that reconcile physical priors with data-driven learning. The work systematically discusses how such models can be fine-tuned for distinct downstream tasks while managing catastrophic forgetting, calibration, and domain shift. Beyond algorithmic concerns, we address the computational infrastructure required to train and serve these large models sustainably, and we interrogate the fairness and representational biases that may emerge from uneven coverage of protein families in training corpora. Governance, policy, and reproducibility frameworks are evaluated alongside deployment scenarios in industrial drug discovery pipelines. By weaving together structural design, system engineering, and regulatory foresight, this paper provides a holistic reference for the next generation of protein electrostatics models, arguing that scientific impact and societal robustness must evolve in tandem with architectural innovation.

Keywords

protein electrostatics; graph foundation models; transfer learning; ionization states; protein stability; molecular graphs; large-scale systems.

1. Introduction

The electrostatic landscape of a protein governs its folding, binding, catalytic activity, and response to environmental conditions. Ionization states of titratable residues, characterized by their pKa values, and the free energy differences that define protein stability upon mutation are two manifestations of the same underlying physical potential. Historically, computational approaches have bifurcated into physics-based continuum electrostatics and empirical structure-based models, each limited by the approximate treatment of solvation and the combinatorial explosion of protonation states. The arrival of highly accurate protein structure prediction engines, prominently AlphaFold2 [1], and the parallel emergence of protein language models that encode evolutionary and biophysical patterns from massive sequence databases [2] have catalyzed a reinterpretation of these classical problems through the lens of geometric deep learning. In this reconfigured landscape, proteins are naturally represented as graphs whose nodes are atoms or residues and whose edges encode spatial proximity and chemical bonding. Graph neural networks operating on such representations, especially those that respect the symmetries of three-dimensional space, have shown remarkable capacity to learn transferable representations of local chemical environments [3].

The challenge of predicting pKa values has seen a progression from the foundational work embodied in empirical tools such as PROPKA [4] through to physics-based treatments rooted in continuum electrostatics [5]. More recently, deep learning methods have been deployed to learn pKa directly from structure, bypassing explicit energy calculations and harnessing the representational flexibility of multi-layer perceptrons and graph architectures. Preprint reports have demonstrated the feasibility of graph-based pKa prediction models that incorporate geometric attention [6], while peer-reviewed studies have established robust benchmarks for deep learning approaches to pKa estimation [7]. A significant direction within this literature involves the infusion of physically derived descriptors such as solvent accessibility, hydrogen bonding networks, and Coulombic interaction fields into graph learning pipelines [8], underscoring the value of hybrid representations that fuse inductive bias with data-driven abstraction.

Protein stability prediction, particularly the estimation of free energy changes due to single or multiple point mutations, has similarly benefitted from deep learning, with architectures ranging from convolutional networks on voxelized structures to graph-based message-passing frameworks [9, 10]. Although these two task families share a common foundation in protein electrostatics, the research communities have remained largely separate, and systematic investigations of transfer learning across ionization and stability domains are sparse. The central thesis of this paper is that a graph foundation model pre-trained on large-scale structural and electrostatic data can serve as a unified backbone for both tasks, enabling positive transfer and reducing the need for task-specific massive labeled datasets. We frame the discussion around system-level considerations, dissecting not only model architecture and training protocols but also the infrastructure, sustainability, fairness, and policy dimensions that accompany the deployment of such models in real-world scientific and industrial contexts.

2. Background and Related Work

Proteins can be parsed as heterogeneous graphs in which nodes carry chemical identities and edges are drawn from spatial proximity thresholds or covalent bonding patterns. When these

graphs are processed by neural networks that respect Euclidean symmetries, such as SE(3)-equivariant message-passing layers, the resulting representations become responsive to the relative orientations of residues while remaining invariant to global rotation and translation. The geometric vector perceptron framework demonstrated the efficacy of this principle in tasks related to protein function and design [3]. Prior to the deep learning era, pKa prediction relied on empirical parameterizations or finite-difference Poisson-Boltzmann solvers. PROPKA3, a widely used method, estimates pKa shifts by evaluating desolvation penalties, hydrogen bonding, and charge-charge interactions using heuristic terms derived from protein structure [4]. Continuum electrostatic models, grounded in the theoretical formalisms reviewed by Honig and Nicholls, provided mechanistic insight but struggled with the heterogeneous dielectric response of proteins in aqueous solution [5]. The limitations of these classical approaches motivated a shift toward machine learning.

The first wave of data-driven pKa prediction trained shallow network regressors on structure-derived features. Subsequent advances replaced handcrafted descriptors with end-to-end learning on atomic point clouds, and later on graphs. A preprint by Gao et al. introduced an equivariant graph neural network that explicitly modeled protonation equilibria while maintaining rotational invariance, achieving promising accuracy on benchmark sets [6]. A separate deep learning approach developed by Unsal et al. systematically evaluated the influence of structural resolution and conformational sampling on pKa prediction, demonstrating that modern architectures can match or exceed physics-based methods when sufficient training data are available [7]. The work that most directly informs the hybrid modeling paradigm integrates physically inspired feature engineering into graph-based learners, enriching node and edge attributes with electrostatic potentials, solvent accessibility metrics, and hydrogen bond propensities [8]. These advances suggest that the integration of domain knowledge can regularize learning and improve generalization to under-sampled regions of sequence space.

For stability prediction, analogous trends are observed. Cao et al. developed DeepDDG, a convolutional neural network that operates on distance maps and physicochemical features to predict folding free energy changes upon mutation [9]. Li et al. introduced PremPS, a method that combines evolutionary information with structural descriptors through an attention mechanism, highlighting the importance of multi-source feature integration [10]. Meanwhile, the field of graph representation learning has produced a suite of pre-training strategies originally demonstrated on molecular graphs. The work by Hu et al. on strategies for pre-training graph neural networks established that masked node and edge prediction tasks can yield representations that transfer across molecular property benchmarks [11]. Contrastive learning on graphs, as formulated by You et al. through graph augmentations, provided an alternative self-supervised objective that promotes robustness to topological perturbations [12]. Extending these ideas to three-dimensional molecular graphs, Liu et al. proposed GraphMVP, a framework that aligns representations derived from 2D topologies and 3D conformations, enabling transfer from geometry-aware pre-training [13]. Despite these advances, a cohesive framework that applies graph foundation model pre-training to the domain of protein electrostatics, and that rigorously evaluates cross-task transfer between pKa and stability, remains absent.

3. Graph Foundation Model Architecture for Protein Electrostatics

Designing a graph foundation model for protein electrostatics begins with the construction of a protein graph that supports both atomic-level fidelity and coarse-grained residue-level views.

At the finest granularity, each heavy atom becomes a node annotated with element type, partial charge from a precomputed force field, and solvent accessibility. Edges are instantiated between atoms within a radial distance cutoff, enriched with interatomic distance encoded by a set of Gaussian radial basis functions and, optionally, angular information to capture the relative orientation of neighboring bonds. To enable the model to reason across scales, a hierarchical architecture can be employed in which atomic messages are first pooled to residue-level embeddings, followed by inter-residue message passing that operates on an alpha carbon trace or on side-chain centroid positions. The architectural backbone is built from equivariant message-passing layers that transform node features under the action of SO(3) or SE(3), preserving directional information essential for modeling anisotropic electrostatic fields. This choice introduces a structural trade-off: while strict equivariance guarantees physical consistency, it increases computational cost and places constraints on the message functions that can be used. Relaxing equivariance through flexible attention mechanisms, such as those found in geometric transformers or vector-attention layers, can boost scalability to large protein systems at the risk of degrading physical fidelity.

The pre-training phase is designed to ingest large-scale corpora of experimentally determined and computationally predicted protein structures, including those from the Protein Data Bank and the AlphaFold Protein Structure Database. A central design question revolves around the selection of pre-training objectives. Masked atom type prediction pushes the model to infer chemical identity from local spatial contexts, implicitly capturing electronegativity patterns and favored coordination geometries that correlate with proton binding. A denoising objective that perturbs atomic coordinates and partial charges and asks the model to reconstruct the original electrostatic potential field can directly encode physics at the level of the Poisson-Boltzmann equation without solving it explicitly. Additionally, a contrastive objective that matches representations of the same local substructure under different protonation microstates serves to embed the chemical equilibria that define pKa values intrinsically in the latent space. The system architect must balance the computational demands of these objectives against their utility for downstream tasks; a pre-training curriculum that escalates from simple atom-level prediction to multi-protonation contrastive learning can mediate this trade-off by allowing cross-task features to accumulate gradually without early overfitting to any single signal.

The governance of such a pre-training pipeline requires careful attention to data provenance and reproducibility. Protein structures derived from different experimental modalities, such as X-ray crystallography, cryo-electron microscopy, and computational prediction, exhibit systematic differences in resolution, thermal factor distributions, and hydrogen atom placement. Pre-training on heterogeneous sources without explicit domain labels risks learning artifacts tied to structure quality rather than genuine electrostatic grammar. Mitigation strategies include domain-adversarial training that penalizes the model for being able to discriminate the origin of a structure, and the injection of metadata as auxiliary inputs that can be gated during fine-tuning. The massive scale of candidate pre-training datasets, which can encompass millions of protein domains, pushes the system into the realm of large-scale distributed training. Parameter synchronization across hundreds of GPU accelerators, combined with data parallelism and pipelining of the graph minibatch assembly, becomes a first-class architectural constraint that interacts with the choice of message-passing radius and model depth.

4. Transfer Learning Paradigms and Task Adaptation

Transferring the pre-trained graph foundation model to the ionization prediction task involves attaching a lightweight readout head that maps residue-level latent representations to scalar pKa values for titratable sites. During fine-tuning, the backbone weights can be partially frozen, allowing only the top few equivariant layers to adjust, or they can be fully updated with a low learning rate and strong weight decay to preserve the pre-trained electrostatic grammar. A critical consideration is that the available pKa training datasets are several orders of magnitude smaller than the pre-training corpus and are heavily skewed toward a limited set of well-studied protein folds. This imbalance makes the fine-tuning stage highly susceptible to catastrophic forgetting of rare chemical environments. Elastic weight consolidation and experience replay with pre-training minibatches interleaved during fine-tuning have been shown to counteract forgetting in vision and language domains, and their adaptation to the irregular topologies of protein graphs constitutes an open engineering challenge with direct implications for predictive reliability across the tree of life. In the context of ionization, transfer is not only from pre-training to fine-tuning but also horizontally across ionizable residue types. A model fine-tuned on aspartate and glutamate pKa data should ideally transfer knowledge to cysteine and histidine without retraining from scratch, because protonation equilibria of different groups are mediated by the same underlying protein dielectric and electrostatic microenvironments. Multi-task architectures that share the backbone and branch into residue-specific readout layers can enforce this inductive bias explicitly, while meta-learning algorithms that structure the fine-tuning episodes as a series of few-shot residues can improve generalization.

Adapting the same foundation model to protein stability prediction poses different demands. Whereas pKa prediction is a per-residue regression task, stability prediction after mutation often requires a global representation that captures the free energy perturbation induced by a single point substitution. The architectural solution involves the addition of a mutation encoder that computes the difference between the representations of the wild-type and mutant sites and then passes this differential signal through a global pooling operation that aggregates context from the entire protein graph. A design decision involves whether to compute the mutation representation in the latent space of the pre-trained model or to augment the input graph with explicit mutant side-chain coordinates generated by a rotamer library and then propagate messages through the full network. The former approach trades chemical accuracy for computational speed and is thus favored for high-throughput virtual screening of deep mutational scans, while the latter is preferable when subtle repacking effects dominate stability. Simultaneous fine-tuning on both pKa and stability data within a shared backbone, using task-specific heads, creates a joint optimization landscape in which gradient conflicts may arise. Strategies such as gradient surgery or uncertainty-weighted loss scaling can dynamically modulate task contributions, ensuring that improvements in ionization prediction are not achieved at the expense of degrading stability performance, and vice versa.

Calibration of the predicted uncertainties is particularly important when these models are integrated into drug discovery decision-making processes. Temperature scaling and isotonic regression applied post hoc to the outputs of the fine-tuned model can correct systematic overconfidence, but these adjustments do not account for the epistemic uncertainty arising from the distributional mismatch between pre-training and target protein families. Bayesian extensions of graph neural networks, implemented via Monte Carlo dropout or via ensembles of independently fine-tuned models, offer a more principled route to capturing epistemic uncertainty while maintaining compatibility with the pre-trained weight initialization. Evaluating the quality of these uncertainty estimates through calibration error metrics on

benchmarks that explicitly stratify by protein fold class and evolutionary depth provides a rigorous framework for understanding the robustness of transfer.

5. Infrastructure, Deployment, and Sustainability

Training a graph foundation model at the scale required to cover the known protein universe is a data center-scale operation. The graph construction pipeline must transform terabytes of structural data into minibatches of variable-sized graphs with tens of thousands of edges, a process that imposes irregular I/O patterns and demands careful design of the data ingestion layer. Frameworks such as TensorFlow and PyTorch, with their distributed data loading and sharding mechanisms, constitute the foundational software infrastructure [14]. Memory footprint is dominated by the storage of edge indices, radial basis function expansions, and intermediate node representations during the forward pass, which drives the adoption of gradient checkpointing and mixed-precision training. In practice, achieving an acceptable throughput requires co-designing the model architecture and the parallelization strategy: the spatial locality of graph convolutions enables domain decomposition across accelerators with minimal cross-partition communication, provided that the protein graphs can be efficiently partitioned using graph clustering algorithms that minimize edge cuts. This co-design imperative is analogous to the challenges faced in large molecular dynamics simulations, but the stochastic optimization loop introduces additional synchronization overhead that must be amortized through gradient accumulation.

The deployment phase for model serving presents a contrasting set of resource constraints. In a typical drug discovery pipeline, a single protein of interest may need to be evaluated for thousands of mutations, requiring the model to process a large batch of related graphs with low latency. Model compilation to optimized inference formats, such as ONNX Runtime with custom graph operators, and quantization of weights and activations can reduce inference time and energy consumption by factors that are critical for cloud-based services. However, aggressive quantization can disproportionately degrade accuracy for rare residue types or edge-case mutations, leading to a tension between computational sustainability and predictive equity. The energy cost of inference across millions of protein variants becomes a material sustainability concern when these predictions are integrated into large-scale virtual screening campaigns. Estimating the carbon footprint of model training and inference following the methodologies advocated by Strubell et al. [15] enables research organizations to make informed decisions about the trade-off between model capacity and environmental impact. Sustainable deployment also encompasses model lifecycle management, including versioning, monitoring for data drift as structural databases grow, and periodic re-training that amortizes the cost of foundation model updates across a consortium of academic and industrial users.

From a governance perspective, the availability of a powerful electrostatic foundation model raises questions about access equity and dual use. If the model is proprietarily hosted or requires expensive GPU infrastructure for fine-tuning, smaller academic labs in low-resource regions may be excluded from participating in the next generation of protein engineering research. Federated pre-training schemes, in which participating institutions contribute model updates without sharing sensitive structural data, could partially alleviate this asymmetry, though they introduce communication overhead and complicate the curation of a globally coherent training dataset. The system design must therefore incorporate not only technical efficiency but also institutional mechanisms for open-weight release, standardized benchmark hosting, and transparent reporting of data composition.

6. Fairness, Bias, and Policy Considerations

Fairness in biomedical machine learning extends beyond demographic parity to encompass the notion that predictive performance should be uniformly robust across the biological diversity that the model is claimed to represent. In the context of protein electrostatics, fairness translates to the ability of the model to make accurate predictions for proteins from poorly annotated organisms, extremophilic environments, and intrinsically disordered regions that are systematically underrepresented in crystallographic databases. A graph foundation model pre-trained predominantly on globular, mesophilic proteins may learn a latent representation of electrostatics that implicitly assumes a narrow range of dielectric responses and solvent configurations. When confronted with a hyperthermophilic enzyme whose stability arises from a dense network of surface salt bridges, the model may systematically mispredict pKa shifts and stability changes, thereby biasing downstream protein engineering efforts toward the sequence space of well-characterized homologs [16]. This form of representation bias can produce a feedback loop: pipelines that rely on the model to filter candidate mutations reinforce the focus on regions where the model is already confident, slowing the discovery of variants with novel electrostatic properties. Mitigating such biases requires deliberate curation of pre-training datasets that span extremophiles, metagenomic sequences, and synthetic protein topologies, combined with evaluation protocols that report performance stratified by phylogenetic distance and structural novelty.

The policy implications of these fairness concerns intersect with regulatory frameworks for machine-learning-guided therapeutic development. If a foundation model is used to prioritize antibody variants for experimental validation, and its electrostatics predictions systematically disadvantage mutations that occur in long, flexible loops or in non-canonical binding interfaces, the resulting candidate pool may inherit a structural blind spot that ultimately reduces therapeutic efficacy or introduces immunogenicity risks. Regulators may require evidence of subgroup performance on a broad panel of protein folds, analogous to the demographic subgroup reporting advocated for clinical prediction models by Rajkomar et al. [17]. This places a burden on model developers to implement continuous monitoring and to release disaggregated performance metrics alongside the model weights. The absence of such transparency could undermine trust in computational pipelines and slow adoption in regulated settings.

Beyond fairness, the broader governance of graph foundation models for proteins must address intellectual property, dual-use concerns, and reproducibility. The pre-training corpus frequently includes structures predicted by third-party models, creating a cascading chain of licenses and usage restrictions that can entangle downstream applications. Clear data provenance tracking and adherence to the FAIR principles for scientific data management [18] are essential to ensure that the model can be ethically distributed and that its predictions are reproducible across different institutional environments. The dual-use risk, wherein the same model that accelerates the development of industrial enzymes could be repurposed to stabilize toxin proteins, necessitates a conversation about access controls and responsible publication practices, albeit without the extreme compartmentalization that would stifle basic research. The ethics frameworks emerging for algorithmic systems, as articulated by Mittelstadt et al., emphasize the importance of foreseeability and stakeholder engagement in shaping such controls [19]. Finally, serving infrastructure must incorporate mechanisms for version-locked reproducibility and explainability. When a clinical candidate fails in late-stage trials, the ability to retrieve the exact model version and feature set that influenced a critical protein engineering decision is indispensable for post-mortem analysis and for maintaining the credibility of the computational methodology.

7. Conclusion

Graph foundation models for protein electrostatics sit at the confluence of geometric deep learning, large-scale systems engineering, and molecular biophysics. This paper has traced the architectural decisions that underpin their design, from equivariant message passing to hierarchical multi-scale graph representations, and has elaborated on the strategies through which transfer learning can unify ionization and stability prediction under a shared pre-trained backbone. We have argued that the success of such models is inseparable from the infrastructure that sustains them, and that the sustainability and fairness challenges they raise must be confronted with the same rigor devoted to algorithmic accuracy. The path forward requires a collaborative ecosystem in which model developers, structural biologists, systems engineers, and policy scholars actively coordinate to ensure that the next generation of electrostatic predictors are not only powerful but also equitable, transparent, and robust across the full expanse of protein space. Only through such integrated scholarship can graph foundation models become reliable instruments for scientific discovery and therapeutic innovation.

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